Course unit descriptions

The data sheets differ from the suggested form in Appendix 1 of the guidelines. We have recently accreditated our MSc in Chemistry programme at the Hungarian Accreditation Committee. We did not rewrite the course sheets from the form presented for the Hungarian accreditation. We hope the Euromaster Label Committee would accept this form, because the rewritten of the 219 sheets and the cross-check with the responsible teachers would be a lot of work and it might cause delay in our application.

Some aspects are not included in our individual data sheets. Fortunately, they are similar in the most of the cases and they are discussed in the self-evaluation report.

Course code The code system will be developed only at the introduction of the training and it will be developed by the administration of the faculty. Now, we do not have any idea about it.

Type of course Lectures, practises or laboratory practices. It could be deduced from the name or the content of the course and it is summarized in the self-evaluation report (tables in section II)

Level of course It is defined by the module: MSc-primary, MSc-specialized or MSc-other sciences or general

Year of study/semester Each course can be chosen in both MSc years, the semesters are unknown yet (see self-evaluation document)

Objective of the course Sorry, it is missing. Maybe it could be deduced from the course content.

Teaching methods Traditional lectures, seminars or laboratory practices (see self-evaluation document)

Assessments methods For the lectures: oral, written or combined exams. For the practices: combined assessment including the quality of reports and work (see self-evaluation)

Language of instruction Hungarian alternates with English yearly (or both, if more than one groups will be present - see self-evaluation).

Table of contents

Semi-optional primary chemical courses

Analytical Chemistry - primary module

Title of the course: Applications of Nuclear Chemistry

Credits: 2

Coordinator: Homonnay, Zoltán

Department: Department of Analytical Chemistry

Prerequisites: Basics of Nuclear Chemistry (KA2MG1) or equivalent.

Topics covered by the course:
Review of the basiscs of nucear chemistry. Nuclear methods in chemical analysis: conventional and prompt gamma neutron activation analysis, gamma spectroscopy, alpha and beta backscattering, XRF, PIXE. Nuclear methods in structural research: Mössbauer-spectroscopy, positronannihilation spectroscopy. Electronspectroscopies. Radiation chemistry. Hot-atom chemistry. Application of radioisotopes in industry. Stable isotopes in nature, application, isotope enrichment methods. Nuclear reactors and energy production. Applications in biochemistry, biology and medicine. Radiation protection.

Literature*:

Compulsory:
Attila Vértes, István Kiss: Nuclear Chemistry, *Akadémiai Kiadó,* Budapest, 1987

Suggested:
Attila Vértes, Sándor Nagy, Zoltán Klencsár: Handbook of Nuclear Chemistry, Kluwer, Amsterdam, 2003
Joseph Magill, Jean Galy: Radioactivity, Radionuclides, Radiation, Springer, Berlin, 2005
G. Choppin, J.O.Liljenzin, J.Rydberg, Radiochemistry and Nuclear Chemistry, Butterworth-Heinemann, 2002.

Title of the course: Applied Analytical Chemistry

Credits: 2

Coordinator: Záray, Gyula

Department: Department of Analytical Chemistry

Prerequisites: admission to Chemistry MSc

Topics covered by the course: analytical techniques for investigation of environmental, food, forensic and drug samples, comparison of their analytical capabilities and evaluation of their harmonization with the requirements of the EU.

Literature:

Compulsory:

Az elemanalitika korszerű módszerei, Szerk.: Záray Gyula, Akadémiai Kiadó, 2006
Applied Spectroscopy, Eds: J. Workman, A. Springsteen, Academic Press, 1998
Handbook of Environmental Speciation I: Techniques and Methodology, Eds.: R. Cornelis, J. Caruso, H. Crews, K. Heumann, Wiley, 2005

Suggested:

Umweltanalytik und Ökotoxikologie, Eds.: S. Holler, C. Schaefers, J. Sonnenberg, Springer, 1996
Fernmessung von Luftverunreinigungen, Ed.: V. Klein, Ch. Werner, Springer-Verlag, 1993

Title of the course: Basics of Nuclear Sciences

Credits: 2

Coordinator: Süvegh, Károly

Department: Deptartment of Analitical Chemistry

Prerequisites: knowledge of math and pfysics at a Chemistry BSc level

Topics covered by the course:
size of the nucleus, mass and charge density of nuclei, nuclear spin and magnetic moment, constituents of nuclei, nuclear force, stable nuclids, nuclear reactions, radioactivity, age determinatio, interactions of radioation and matter, detectors, nuclear reactors

Literature*:
Suggested books:
Vértes, A., Kiss, I.**:** Nuclear Chemistry, *Elsevier*, Amsterdam, 1987
K.S. Krane: Introductory Nuclear Physics, *Wiley*, New York, 1987
B. Martin: Nuclear and Particle Physics, Wiley, New York, 2006

Title of the course: Chemical Analysis of Air and Water Environments

Credits: 2

Coordinator: Salma, Imre

Department: Department of Analytical Chemistry

Prerequisites: Environmental Chemistry or equivalent knowledge

Topics covered by the course:

General process of environmental pollution, imission, and transmission, classification of the pollution sources of and main pollutants in the air and waters, hazard represented by the main pollutants.

Sampling methods for gases and aerosol particles. Laboratory and on-line measuring methods for atmospheric gasses and aerosols. International and national legislations. Methods of reducing air pollution.

Water management. Water pollution, main polluting species. Sampling and qualification tests of surface-, ground- and undersurface (aquifer) waters. Water quality maps. WHO, EU recommendations, national standards. Water purification and treatment technologies. International legislation on diminishing pollutants.

Literature:

Compulsory:

Manahan, S.E., Environmental Chemistry, 6th or 7th ed., Lewis, Boca Raton, 1994.

Suggested:

Finlayson-Pitts, B.J., Pitts, J.N., 1990. Atmospheric Chemistry: Fundamentals and Experimental Techniques, Wiley
Ligetvári Ferenc: Környezetünk és védelme 3. kötet, Vízminősítés, vízkezelés könyvfejezet, 9-128 oldal, Ökológiai Intézet a Fenntartható Felődésért Alapítvány, Miskolc, 2000.

Title of the course: Instrumental Analysis Lab (2)

Credits: 4

Coordinator: Zihné Perényi, Katalin

Department: Department of Analytical Chemistry

Prerequisites: Instrumental Analysis I. or equivalent knowledge and practice

Topics covered by the course:
Thermo analysis. Application of differential scanning calorimetry (DSC) in polymer study. Determination of Ca-oxalate and Ca carbonate by thermogravimetry. Electro analysis. Determination of Pb^{2+} / Cd^{2+}- ions by differential pulse anodic stripping voltammetry (DPSV) in anal. grade $NaNO_3$. Atomic spectrometry. Determination of As\Se contamination in soils coupling hydride generation to inductively coupled plasma atomic emission spectrometry (HG-ICP-AES). Selective leaching of cave sediment and determination of its Pb\Cu content by graphite furnace atomic absorption spectrometry (GFAAS). Chromatography. Determination of trace organic contaminants in Danube water by gas chromatography and mass spectrometric detection (GC-MS).
Interpretation of some high efficiency analytical techniques by interactive teaching software. On-line operation of instruments and off-line evaluation of data.

Literature*:
Compulsory:
http:\\anal.chem.elte.hu
Suggested:
R. Kellner, J.M. Mermet, M.Otto, H.M. Widmer Analytical chemistry, Wiley, 1998

Title of the course: Investigation Methods of Material Structures B: supramolecular scale

Credits: 2

Coordinator: Sinkó, Katalin

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in instrumental analytical and physical chemistry

Topics covered by the course:

Investigation methods of material structures in supramolecular ranges

Light scattering **(**theory of static and dynamic light scattering, determination of diffusion standards and sizes of particles); X-ray- and neutron scattering, SAXS and SANS (supramolecular structural investigations of amorphous materials with small and wide angle X-ray and neutron scattering, theories of X-ray and neutron scattering, comparison of SAXS and SANS, evaluation of scattering pattern, SAXS, SANS investigation of amorphous and some ordering showing materials); Electron and neutron diffractions (theories, instruments, neutron sours and detectors, application possibilities).

Morphological and surface investigation methods

Electronmicroscope (theories and operational principles of scanning and transmission elecetronmicroscope)**;** Scanning and atomic force microscope, AFM, STM (morphology of solid surfaces, phase structures of composite materials, determination of elastic modules, investigation of solid-liquid interfaces); Surface analysis, XPS (nanolayers atomic analysis, chemical structures, dept profile analysis)**;** Reflection optical methods, ellipsometry, reflectometry, OWLS, SPR, direct force measurements (optical theories of methods, determinations of layer thickness, molecule orientations, microstructures, and crystalline structures, applications as sensors)

Literature:

P. Lindner, Th. Zemb (eds): Neutron, X-Ray and Light Scattering, North-Hollnad, Oxford, 1991.

Title of the course: Laboratory Practice on Separation Methods

Credits: 4

Coordinator: Torkos, Kornél

Department: Deptartment of Analytical Chemistry

Prerequisites: a course on separation techniques

Topics covered by the course: Sampling preparation methods, applications of hyphenated techniques, validation methods, special injection techniques.

Literature:
Compulsory: Daniel R.Knapp Analytical Derivatization Reactions
Walter Jennings Analytical Gas chromatography

Suggested Jan:usz Pawliszin Solid Phase Microextraction (Theory and Practice)

Title of the course: Separation Techniques

Credits: 2

Coordinator: Torkos, Kornél

Department: Deptartment of Analytical Chemistry

Prerequisites: the basics of physical-chemistry

Topics covered by the course: special detection techniques in gas and fluid chromatography, applications for environment food and pharmaceutical samples. Sample preparation and sample handling processes Hyphenated techniques (GC-MS, HPLC-MS)

Literature: Stanley Manahn Environmental Chemistry
WalrerJennings Analytical Gas Chromatography
Daniel R. Knapp Analytical Derivatization Reactions

Compulsory:

Suggested:
Sample Preparation for Gas Chromatography
Encyclopedia of Analytical Chemistry: Instrumentation and Applications
R.A. Meyers (Ed.)
John Wiley & Sons Ltd, Chichester, 2000 pp 10723-10730

Inorganic Chemistry - primary module

Title of the course: Applied organometallic chemistry

Credit: 2

Coordinator /Department: András Kotschy associate professor, Department of Inorganic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in inorganic and organic chemistry (successful exams in inorganic and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Fundamentals of organometallic chemistry, structure and reactivity of polar organometallic reagents, sodium and potassiumorganic reagents in organic synthesis, lithiumorganic reagents in organic synthesis, magnesiumorganic reagents in organic synthesis, superbases, zincorganic reagents in organic synthesis, tinorganic reagents in organic synthesis, organocopper reagents in organic synthesis.

Compulsory literature*:
Faigl F., Kollár L., Kotschy A., Szepes L. Szerves fémvegyületek kémiája, *Nemzeti Tankönyvkiadó*, Budapest, 2001

Suggested literature:
A. Kotschy, G. Timári, Heterocycles from Transition Metal Catalysis, *Springer*, 2005

Title of the course: Bioinorganic chemistry

Credits:2

Coordinator/Department: Olti-Varga Margit, associate professor

Department of Analytical Chemistry

Terms for joining: beginning terms of the Chemistry Msc., basic knowledge in inorganic and analytical chemistry (successful exams from inorganic, analytical and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Attainment of contemplation of bioinorganic chemistry: approach and explanation of chemical, biological, biochemical and medical questions by taking into consideration of different aspects. Demonstration of multiple connection of geological and biological environment. Presentation of the role of essential and toxic elements in living organism on molecular level.

Literature:
Compulsory: -
Suggested:
Endre Kőrös: Bioinorganic chemistry (lecture notes)
W. Kaim, B. Schwederski: Bioinorganic chemistry, Wiley, 1994

Title of the course: Catalysis lab

Credit: 4

Coordinator /Department: András Kotschy associate professor, Department of Inorganic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in inorganic and organic chemistry (successful exams in inorganic and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
reactions in inert media, fundamentals of catalysis, the analytical tracking of catalysis (TLC, GC, HPLC, NMR), heterogeneous catalysis, homogeneous catalysis, asymmetric synthesis, cross-coupling reactions, metathesis, hydrogenation, kinetic study of catalytic processes

Compulsory literature*:
Faigl F., Kollár L., Kotschy A., Szepes L. Szerves fémvegyületek kémiája, *Nemzeti Tankönyvkiadó*, Budapest, 2001

Suggested literature:
A. Kotschy, G. Timári, Heterocycles from Transition Metal Catalysis, *Springer*, 2005

Title of the course: Laboratory Excercises of Modern Structural Research Methods

Credits: 4

Coordinator/Department: Dr. János Rohonczy / Department of Inorganic Chemistry

Terms for joining: Fulfilment of the course "Modern Structural Research Methods"

Topics covered by the course:
The aim of this course is the experimental introduction to the most important, modern structural research methods, i.e. IR-, Raman-, UV-, photoelectron and NMR spectroscopy, mass spectrometry and X-ray diffraction as well as GC and HPLC separation technique. During this course students learn the main parts of the instruments, the sample preparation, data acquisition and processing techniques. Some typical real examples are used to demonstrate the ability of the mentioned experimental methods.

Literature*:
Compulsory:

Suggested:

P.J. Hore: Nuclear Magnetic Resonance, Oxford University Press, 1995. (ISBN13: 9780198556824, ISBN10: 0198556829)
Kovács I., Szőke J.:Molekulaspektroszkópia, Akadémiai Kiadó, Budapest, 1987.
Colin F. Poole and Salwa K. Poole: Chromatography today (Elsevier, 1991)

Title of the course: Modern structural research methods

Credits: 2

Coordinator/Department: Dr. János Rohonczy / Department of Inorganic Chemistry

Terms for joining: entry criteria of MSc. in chemistry

Topics covered by the course:
The aim of this course is to introduce the instruments and the relating methods of the most important, modern structural research, as IR-, Raman-, UV-, photoelectron and NMR spectroscopy, mass spectrometry and X-ray diffraction. GC and HPLC separation technique as the parts of the most important GC-MS and HPLC-NMR coupled methods are also discussed. This course focuses on the experimental methodology, the theoretical backgrounds and the typical application fields of all aforesaid methods as well. The presentation of "find a method to the problem" is discussed through samples from the practice.

Literature*:
Compulsory:

Suggested:

P.J. Hore: Nuclear Magnetic Resonance, Oxford University Press, 1995.
(ISBN13: 9780198556824, ISBN10: 0198556829)
Kovács I., Szőke J.:Molekulaspektroszkópia, Akadémiai Kiadó, Budapest, 1987.

Title of the course: Organometallic and Catalysis Laboratory Course

Credits: 5 credits

Coordinator/Department: László Szepes Professor in Chemistry

Deparment of Inorganic Chemistry

Terms for joining: general entrance requirements of Chemistry MSc program, basic knowledge

in Organometallic and Preparative Organic Chemistry. (In the case of completed ELTE BSc

courseprerequisites are Organometallic Chemistry (kv1n1en5) and Organic Chemistry Lab 1

(kv1n4es3), or equivalent in any other case.)

Topics covered by the course:
In course of the laboratory practice the students get experience in the field of advanced preparative and manipulation techniques like semi-micro syntheses in vacuum and inert atmosphere, the Schlenk technique, electro- and photochemical preparations, microwave assisted reactions, chemical vapour deposition. The studied chemical systems include – among others – transition metal catalysts, clusters, organometallic reagents and precursors.

Literature:
The manual containing experimental procedures together with discussion and brief theory is available via internet (Hung.).

Faigl Ferenc, Kollár László, Kotschy András, Szepes László: Szerves Fémvegyületek Kémiája, Nemzeti Tankönyvkiadó, Budapest, 2001., I.-III. fejezet (Hung.)

Ch. Elschenbroich, A Salzer: Organometallics, VCH, Weinheim, 1992. (Eng.)

Title of the course: Organometallic Chemistry

Credits: 2 credits

Coordinator/Department: László Szepes Professor in Chemistry

Department of Inorganic Chemistry

Terms for joining: general entrance requirements of Chemistry MSc program, basic knowledge

in Inorganic and Organic Chemistry. (In the case of completed ELTE BSc prerequisites are

Inorganic Chemistry 1 (kv1n1en1) and 2 (kv1n1en2), as well as Organic Chemistry 1 (kv1n1es1)

and 2 (kv1n1es2), or equivalent in any other case.)

Topics covered by the course:
The course intends to provide the students with the definitions and basic principles of organometallic chemistry, its history and its position in chemistry, the main trends in research and applications. Further topics as the nature of the metal-carbon bond, the basic groups of compounds, stability and thermochemistry, preparation as well as characteristic reactions are discussed. Typical examples concerning structure and bonding, as well as industrial applications are shown.

Literature:
Faigl Ferenc, Kollár László, Kotschy András, Szepes László: Szerves Fémvegyületek Kémiája, Nemzeti Tankönyvkiadó, Budapest, 2001., I.-III. fejezet (Hung.)
Ch. Elschenbroich, A Salzer: Organometallics, VCH, Weinheim, 1992. (Eng.)

Title of the course: Structural Chemistry

Credits:

Coordinator/Department: Antal Csámpai / Department of Inorganic Chemistry

Terms for joining: Successful exams: Inorganic Chemistry, Organic Chemistry, Theoretical Chemistry

Topics covered by the course: The basic concepts of the most important methods of structure determination and the scope and limitations of their application in inorganic chemistry. Structure and reactivity of simple and more complex inorganic compounds, recognition of synthetic possibilities on the basis of structural considerations taking into account eg. the principle of isolobality, with special regard to borane-, carborane-, metallocarborane- and metal clusters. The application of different levels of theory of chemical bonding to interpret the structure of more complex inorganic compounds.

Literature*:

Compulsory:

N. N. Greenwood, A. Earnshow: Az elemek kémiája I-III. Nemzeti Tankönyvkiadó RT Budapest 1999.

Suggested:

Purcell-Kotz: Inorganic Chemistry

F. Cotton, G. Wilkinson: Advanced Inorganic Chemistry (John Wiley & Sons, 1992.)

Csákvári Béla és Pongor Gábor, Az átmenetifémek és fémorganikus vegyületek sztereokémiája (A kémia újabb eredményei 1998, Akadémiai Kiadó)

Bodor E., Papp S.: Szervetlen Kémia (Tankönyvkiadó, 1983.)

Organic Chemistry - primary module

Title of the course: Biochemistry

Credit: 2

Coordinator /Department: Zoltán Gáspári / Department of Organic Chemistry

Terms for joining: Organic chemistry

Topics covered by the course:

Molecular organization of life. The central dogma. Basics of metabolism and metabolic pathways. Protein structure and function. Basic enzyme kinetics and mechanisms. Regulation of gene expression. Biochemistry of sensory systems. Introduction to basic experimental techniques.

Compulsory literature:
Berg-Tymoczko-Stryer: Biochemistry 5th ed.

Suggested literature :
Bálint Miklós: Molekuláris biológia I-II-III.,

Title of the course: Biomolecular chemistry I

Credit: 2

Coordinator /Department: Miklós Hollósi professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and natural products chemistry (successful exams in organic chemistry and biochemistry; for others: equivalent knowledge)

Topics covered by the course:
The molecular design of life. Biochemical reactions, cofactors and transport molecular. Proteins, enzymes. Chemistry of nucleic acids, building blocks of DNA and RNA, structure of DNA and RNA. Biological role of DNA and RNA, transcription, translation, targeting of proteins. Exploring evolution, bioinformatics

Compulsory literature*:
M. Hollósi., L. Laczkó, B. Asbóth, Biomolekuláris kémia I, Nemzeti Tankönyvkiadó, Budapest, 2005

Suggested literature:
M. Hollósi., B. Asbóth, Biomolekuláris kémia II, Nemzeti Tankönyvkiadó, Budapest, 2007

Title of the course: Green chemistry

Credit: 2

Coordinator /Department: István T. Horváth, Professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc. and basic knowledge in inorganic and organic chemistry (successful exams in inorganic and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
The rapidly increasing worldwide demand for environmentally friendly chemical products and processes requires the application of novel and cost-effective technologies to pollution prevention. Green Chemistry is an emerging new approach focusing on a simple principle that it is better to prevent waste than to treat or clean up waste after it is formed.
Topics:
The Fundamentals of Green Chemistry
The Chlorine Controversy
Replacing Toxic Chemicals
Alternative Solvents and Reaction Media
Selective Catalysis
Asymmetric Synthesis
Energy and the Environment
Population and the Environment
Environmental Economics
The Environmental Factor in Chemical Research and Development Management

Compulsory literature*:
P.T.Anastas, J.C. Warner: Green Chemistry, Oxford University Press, Oxford, 1998
Suggested literature:

Name of course: Green Chemistry Laboratory Practice

Credits: 4

Coordinator: István T. Horváth, Professor, Department of Oragnic Chemistry

Terms for joining: requirements of the Chemistry MSc. and basic knowledge in inorganic and organic chemistry (successful exams in inorganic and organic chemistry, for others: equivalent knowledge)

Topics covered by the practice:

The course provide advanced training on the fundamentals and applications of green chemistry:

Halogenation of alkenes
Dehydration of alcohols
Synthesis of cyclohexane and adipic acid
Porphyrine synthesis
Microwave assisted synthesis
Diels-Alder reaction
Bioethanol synthesis
Benzoin condensation
Pechman reaction
Sun-light conversion

Compulsory literature:

For details see http://www.greenchemistry.chem.elte.hu/

James E. Hutchington, Kenneth M. Doxee; Green Chemistry in Education Workshop (University of Oregon)

K. L. Williamson, Macroscale and Microscale Organic Experiments, 2nd Ed. 1994, Houghton Mifflin

Suggested literature:

P.T.Anastas, J.C. Warner: Green Chemistry, Oxford University Press, Oxford, 1998

Title of the course: Organic chemistry 3

Credit: 2
Coordinator /Department: Dénes Szabó associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exams in organic chemistry, for others: equivalent knowledge)

Topics covered by the course: Structural features and synthesis of aliphatic, aromatic and heteroaromatic compounds. Mechanism of substitution, addition and rearregements reactions. Stereochemical features of organic reactions. Stereospecific and asymmetrical syntheses. Important organic reactions in the industrial chemistry. Chemical literature.

Suggested literature:

Bruckner Győző: Szerves kémia I-III, Tankönyvkiadó

J. March: Advanced organic chemistry, John Wiley and Sons

R.T. Morrison, R.N. Boyd: Organic chemistry, Allyn and Bacon, Inc.

Title of the course: Organic chemistry laboratory 3

Credit: 4

Coordinator /Department: József Rábai associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in inorganic and organic chemistry (successful exams in inorganic and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Design and practice of complex organic synthesis based on literature search. Safe manipulation with hazardous reagents and use of methods allowing effective separation of synthesis products (liquid chromatography, gas chromatography, crystallizations, sublimation, liquid-liquid extractions). Purity evaluation with spectroscopic methods (UV, FTIR, MS, and NMR).

Compulsory literature*:
(1) Szerves Kémiai Praktikum, Szerk.:Orosz György,Nemzeti Tankönyvkiadó, Budapest, 1998.

Suggested literature:
(1) Vogel's Textbook of Practical Organic Chemistry; Longman Scientific & Technical, UK and John Wiley & Sons Inc. N.Y. 1989.
(2) Natural Products, Raphael Ikan, Academic Press London and New York, 196 1979.

Name of the course: Organic spectroscopy

Credit: 2

Coordinator/Department: Elemér Vass, associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry [successful exam in organic chemistry (2), for others: equivalent knowledge]

Topics covered by the course:
The course covers the theoretical aspects of some of the most important spectroscopic methods used in the structure investigation of organic compounds such as UV-visible, infrared, electronic and vibrational circular dichroism (CD and VCD), NMR and mass spectrometry, with special emphasis to the structure elucidation based on complex spectral evaluation.

Compulsory literature:
Joseph B. Lambert, Herbert F. Shurvell, David A. Lightner, R. Graham Cooks: Organic Structural Spectroscopy, Prentice Hall, Upper Saddle River, New Jersey, USA (2001).

Suggested literature:
Ruff Ferenc: Szerves vegyületek szerkezetvizsgálata spektroszkópiai módszerekkel – Infravörös spektroszkópia, jegyzet, Eötvös Loránd Tudományegytem, Természettudományi kar, Tankönyvkiadó, Budapest (1991).

Ruff Ferenc: Szerves vegyületek szerkezetvizsgálata spektroszkópiai módszerekkel – Ultraibolya spektroszkópia, jegyzet, Eötvös Loránd Tudományegytem, Természettudományi kar, Tankönyvkiadó, Budapest (1991).

Hollósi Miklós, Laczkó Ilona, Majer Zsuzsa: A sztereokémia és kiroptikai spektroszkópia alapjai, Nemzeti Tankönyvkiadó, Budapest (2003).

L.D. Field, S. Sternhell, J.R. Kalman: Organic Structures from Spectra, third edition, John Wiley & Sons, Chichester, UK (2002).

Title of the course: Organic spectroscopy laboratory

Credit: 4

Coordinator/Department: Elemér Vass, associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and spectroscopy [successful exams in organic chemistry (2) and organic spectroscopy, for others: equivalent knowledge]

Topics covered by the course:

The aim of the course is to teach students the most important instrumental methods used in the structural investigation of organic compounds and biomolecules. Besides learning the basic methodology, the students are performing complex measurements which reveal the applicability and limitations of the studied analytical methods. The wide range of covered investigation techniques is aimed at developing the critical sense of students in choosing the most appropriate analytical procedure for solving a concrete problem and to be able to determine the structure of an unknown compound by combining several structural analysis methods. The course also gives an introduction to the stereochemical structure analysis of biomolecules.
The subject includes ultraviolet-visible (UV-VIS), infrared (IR), NMR, circular dichroism (CD), as well as organic and biomolecular mass spectrometry laboratory courses.

Compulsory literature:
Műszeres Szerves Analitikai Gyakorlatok, Egyetemi jegyzet, összeállította az ELTE Szerves Kémiai Tanszék munkaközössége, Budapest (1995).
Joseph B. Lambert, Herbert F. Shurvell, David A. Lightner, R. Graham Cooks: Organic Structural Spectroscopy, Prentice Hall, Upper Saddle River, New Jersey, USA (2001).
Suggested literature:
Ruff Ferenc: Szerves vegyületek szerkezetvizsgálata spektroszkópiai módszerekkel – Infravörös spektroszkópia, jegyzet, Eötvös Loránd Tudományegytem, Természettudományi kar, Tankönyvkiadó, Budapest (1991).
Ruff Ferenc: Szerves vegyületek szerkezetvizsgálata spektroszkópiai módszerekkel – Ultraibolya spektroszkópia, jegyzet, Eötvös Loránd Tudományegytem, Természettudományi kar, Tankönyvkiadó, Budapest (1991).
Hollósi Miklós, Laczkó Ilona, Majer Zsuzsa: A sztereokémia és kiroptikai spektroszkópia alapjai, Nemzeti Tankönyvkiadó, Budapest (2003).
L.D. Field, S. Sternhell, J.R. Kalman: Organic Structures from Spectra, third edition, John Wiley & Sons, Chichester, UK (2002).

Title of the course: Polymer chemistry and technology lab

Credit: 4

Coordinator /Department: Béla Iván, MTA KKI

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and chemical technology (successful exams in organic chemistry and chemical technology, for others: equivalent knowledge)

Topics covered by the course: Literature search and evaluation by the use of computers and the internet databases, synthesis and modification of polymers on the basis of literature processes, analysis of polymeric materials by FTIR, NMR, DSC, gel permeation chromatography (GPC) for determining molecular weight distribution, report writing on the accomplished lab work

Compulsory literature: Handouts provided during the course

Suggested literature:

Title of the course: **Theoretical organic chemistry**

Credits: **2 lectures / week , 2 credit**
Credit number: **2**

Coordinator: **Perczel András**

Department: **Organic Chemistry**

Closing the course: **colloqium**

Topics covered by the course:

- Short overview of computational methods and possibilities in theoretical organic chemistry outlining briefly the theoretical background of semi-empirical, *ab initio*, post-Hartree-Fock and dft methods.
- Details of basic organic reaction types: comparison of computed and experimentally determined values and parameters.
- Various aspects of typical or basic organic reactions: Electrophilic addition, Nucleophilic addition, Aromatic electrophilic substitution, Nucleophilic substitution, Electrophilic elimination, Nucleophilic elimination and Diels-Alder addition, *etc*..
- Further topics to be covered: calculation of solvent effect, vibrational- and NMR-parameters, proton affinity and pK values, *etc*..
- Comprehensive study of complex systems.

Compulsory literature: lecture notes will be available as the course begins

Suggested literature:
Collection of figures and notes in organic chemistry (edited at the Department),
T. W. Graham Solomons, Craig B. Fryhle: *Organic Chemistry* ISBN 0-471-19095-0,
L. G. Wade, Jr.: *Organic Chemistry* ISBN 0-13-922741-5
Bruckner Győző: Szerves Kémia I-III.

Physical Chemistry - primary module

Title of the course: Advanced Physical Chemistry Laboratory

Credits: 4

Coordinator/Department: Győző G. Láng, professor , Institute of Chemistry, Department of Physical Chemistry

Terms for joining: Basic knowledge in mathematics, physics and physical chemistry. Prerequisites are Physical chemistry laboratory (1) and Physical chemistry laboratory(2), or their equivalents.

Topics covered by the course:
The goal of the labs is to gain familiarity with a variety of physicochemical measurement techniques. Following objectives are pursued: To apply the principles of thermodynamics, kinetics and electrochemistry presented in the physical chemistry lecture courses, and to perform highly complex, advanced level experiments using various advanced techniques. To understand better the interconnection between experimental foundation and underlying theoretical principles and to appreciate the limitations inherent in both theoretical treatments and experimental measurements. The main topics are: Phase and chemical equilibria in highly complex physicochemical systems. Determination of dielectric and magnetic properties. Spectrophotometry in the IR, VIS, and UV region. Methods for the determination of the refractive index. Polarimetry. Complex electrochemical measurements (investigation of electrode processes with complex reaction kinetics with the help of rotating disc electrode, impedance spectroscopy). Scanning tunneling microscopy. Analysis of noise.

Literature*:
Garland, C.W., Nibler, J.W, Shoemaker, D.P.,: Experiments in Physical Chemistry, McGraw-Hill, New York, 2002. Wayne R.P.: Chemical Instrumentation, Oxford 1995.
Caria, M.: Measurement Analysis, Imperial College Press, London, 2000.
Szalma, J., Láng, G., Péter, L.: Fundamental methods in the physical chemistry laboratory – measurements and data processing (English version in preparation)
Recommended:
Böttcher C.J.F.: Theory of Electric Polarization, Amsterdam (1973); A. J. Bard: Instrumental Methods in Electrochemistry, New York (2001.);

Title of the course: Computational chemistry

Credits: 2 + 2

Coordinator/Department: Gergely Tóth, Physical chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
The computational practice follows the topics of the lectures. Different software packages will be used in the practice.
Data processing, interpolation, smoothing, derivation, integration, Fourier transformation, reaction kinetic calculations, modeling of condensed phases with Monte Carlo and classical dynamics, quantum mechanical calculations, modeling of biomolecules, computer aided drug research

Literature*:
Compulsory: Notes on internet in progress
Suggested: Baranyai A, Schiller Róbert, Statisztikus mechanika vegyészeknek ,Akadémiai, 2003.
Valkó P. és Vajda S.: Műszaki–tudományos feladatok megoldása személyi számítógéppel, Műszaki, 1987.
Veszprémi Tamás, Fehér Miklós: A kvantumkémia alapjai és alkalmazása, Műszaki, 2002.
Frank Jensen: Introduction to Computational Chemistry, Wiley, 1999.
Kémia újabb eredményei 80. kötet, Akadémiai, 1995.

Title of the course: Computer Laboratory A

Credits: 0+4

Coordinator/Department: Géza Fogarasi, Inorganic Chemistry

Prerequisites: at least two semesters of physical chemistry and one semester of theoretical chemistry

Topics covered by the course:
A: Molecular structures, reaction mechanisms and molecular modeling of biologically relevant systems
The use of commercial computer programs in molecular research. Quantum chemical calculations at semiempirical and ab initio levels: molecular orbitals,electronic structure; optimization of molecular geometries; computation of vibrational frequencies, infrared and Raman spectra. Electric and magnetic properties, nuclear magnetic resonance (NMR) spectra. Study of reaction mechanisms, transition states, relative energies. Isomers and conformers of biomolecules.

Literature*:
Compulsory:
Frank Jensen: Introduction to Computational Chemistry, John Wiley & Sons, Chichester, New York; 1999. ISBN: 0 471 98425 6.
Suggested:
Christopher J. Cramer: Essentials of Computational Chemistry, John Wiley & Sons, Chichester, 2002. ISBN: 0 471 48552 7.
Errol Lewars: Computational Chemistry, Kluwer Academic, Boston/Dordrecht/London, 2003. ISBN: 1-4020-7285-6.

Title of the course: Computer Laboratory B

Credits: 0+4

Coordinator/Department: András Baranyai, Physical Chemistry

Prerequisites: at least two semesters of physical chemistry and one semester of theoretical chemistry

Topics covered by the course:
B: Statistical mechanical simulations, modeling in reaction kinetics
Simulation methods based on classical statistical mechanics: Monte Carlo and molecular dynamics methods. Molecular mechanics. Mixed classical/quantum simulations, reaction dynamics. Mesoscopic simulations. Modeling in reaction kinetics.

Literature*:
Compulsory:
Suggested:
Baranyai A., Schiller R., Statisztikus mechanika vegyészeknek (Akadémiai, 2003)
Frank Jensen: Introduction to Computational Chemistry, John Wiley & Sons, Chichester, New York; 1999. ISBN: 0 471 98425 6.
Christopher J. Cramer: Essentials of Computational Chemistry, John Wiley & Sons, Chichester, 2002. ISBN: 0 471 48552 7.
Errol Lewars: Computational Chemistry, Kluwer Academic, Boston/Dordrecht/London, 2003. ISBN: 1-4020-7285-6.

Title of the course: Dielectric, magnetic and optical properties of the materials

Credits: 2

Coordinator/Department: László Túri, Department of Physical Chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
Consistent treatment of the electric (dielectric), magnetic and optical properties of the materials based on microscopic and macroscopic principles
Introduction to classical and quantum electrodynamics
Electric properties: electric polarization, electric dipole moment, polarizability, relative permittivity
Magnetic properties: magnetic polarization, magnetic susceptibility, paramagnetism, magnetic resonance parameters
Optical properties: polarization, interference, diffraction, optical activity, refractive index
Introduction to non-linear optics

Compulsory*:
Lecture notes on the internet (in preparation)
Suggested:
Mai fizika, R.P. Feynman, R.B. Leighton, M. Sands, Műszaki Könyvkiadó, Bp.1970
Budó Ágoston, Kísérleti Fizika I-III, Tankönyvkiadó, 1985
P. W. Atkins: Fizikai Kémia II. Szerkezet, Nemzeti Tankönyvkiadó, 2002
P. W. Atkins, R. S. Friedman: Molecular Quantum Mechanics, Oxford University Press, 1997
Kaposi Olivér szerk.: Bevezetés a fizikai kémiai mérésekbe I-II., Tankönyvkiadó

Tantárgy neve: Electrochemistry

Credits: 3

Tantárgyfelelős neve/tanszéke: György Inzelt,

Department of Physical Chemistry

Előtanulmányi feltételek: Physical chemistry

Az elsajátítandó ismeretanyag rövid (néhány soros) leírása:
The development and importance of electrochemical concepts, investigation methods and technologies. Thermodynamical description of homogeneous and heterogeneous electrochemical systems. The structure of the electrochemical double layer. Kinetics of electrochemical processes. Electrochemical methods. Spectroelectrochemistry. Techniques for the investigation of surfaces. Electrosorption. Electrocatalysis. Organic electrochemistry. Photoelectrochemistry. Electrochemical technologies. Enviromental electrochemistry. Electrochemical sensors.

Kötelező irodalom*: Electroanalytical Methods (ed. F. Scholz), Springer, 2002.
A.J. Bard, L.R. Faulkner: Electrochemical Methods, Wiley, 2000.
Selected papers and reviews
Ajánlott irodalom: *C.M.A. Brett, A.M.Oliveira-Brett: Electrochemistry, Principles, Methods and Applications, Oxford Univ.Press, Oxford, 1993; E.Gileadi: Electrode Kinetics, VCH, 1993*

Title of the course: Electronic structure of molecules

Credits: 2 + 0

Coordinator/Department: Prof. Péter Szalay, Physical Chemistry

Terms for joining: Mathematics for Chemists, Quantum Mechanics

Topics covered by the course:
Electronic structure of atoms, atomic orbitals, atomic spectra; Electronic structure of diatomic molecules, the concept of molecular orbitals; MO theory, Hartree-Fock methods; Electronic structure of general molecules, Valence Bond theories; Electronic structure of conjugated molecules, Hückel-theory; Electronic structure of transition metal complexes, crystal field and ligand field theories; Electronic structure of periodic systems; bend structure, Brillouin zone, conduction, semi-conduction, isolation; Methods of electronic structure theories.

Literature*:
Compulsory: Notes on internet in progress
Török F. és Pulay Péter: Elméleti Kémia I, Nemzeti Tankönyvkiadó, 1994.
P. W. Atkins: Fizikai Kémia II. Szerkezet, Nemzeti Tankönyvkiadó, 2002
Suggested:
Peter Attkins és Ronald Freidman: Molecular Quantum Mechanics, Oxford University Press, 2005

Title of the course: Interactions in colloid and nanosize systems

Credits: 2

Coordinator/Department: Tibor Gilányi, Physical chemistry

Terms for joining: Basic knowledge in colloid and surface chemistry

Topics covered by the course:
Excess interfacial energy and its consequences.
Gibbs thermodynamics of interfaces.
Adsorption on different interfaces, adsorption isotherms, surface equation of state.
Electrical structure of solid/liquid interfaces (Gouy-Chapman theory).
Interactions in colloid and nanosize systems, stability.
Theories of colloid stability.
Interfaces and colloid systems in external fields.

Literature*:
Compulsory: Notes on internet in progress
Suggested: Wolfram Ervin, Kolloidika, I., II/1, jegyzet, Tankönyvkiadó, Budapest, 1989.
D. J. Shaw: Bevezetés a kolloid- és felületi kémiába. Műszaki Könyvkiadó, Budapest, 1986
R. J. Hunter: Foundation of Colloid Science, Clarendron Press, Oxford, 1993

Title of the course: Interfacial chemistry

Credits: 2

Coordinator/Department: Kiss, Éva, associate professor Department of Physical Chemistry

Terms for joining: beginning terms of the Chemistry MSc., basic knowledge in colloid and surface chemistry (for those having an ELTE chemistry Bsc.: Basics of Colloid and Surface Chemistry, KA2KL1 and KA2KL2; for others: equivalent knowledge)

Topics covered by the course:

Natural and synthetic surface active agents, their impact on the enviroment. Surface active polymers. Polymer and polyelectrolyte surfactant complexes.
The surface and interfacial interactions, measuring techniques. Surface modification methods.
Structure of surface nanolayers. Ordered molecular films: SA, Langmuir and LB. Thin liquid films. Interfacial rheology, shear and dilatational parameters.
Monodisperse colloidal systems. Foams, emulsion, microemulsions. Microgels. "Intelligent materials". Heterocoagulation (interaction between various surfaces).
Separation techniques in the colloid dimensions. Macro- and micro-flotation.

Literature*:

Compulsory:

F. McRitchie: Chemistry at Interfaces, Academic Pr. London, 1990.
K. Tsujii: Surface Activity, principles, phenomena and applications, Academic Pr., San Diego, 1998.
B. Jönsson, B. Lindman, K. Holmberg, B. Kronberg: Surfactants and polymers in aqueous solutions, Wiley, Chichester, 1998.
H. Lyklema: Fundamentals of Interface and Colloid Science, vol III, Academic Pr., San Diego, 2000.

Suggested:

J. Israelachvili: Intermolecular and Surface Forces, Academic Pr., London, 1992.

Title of the course: Modern investigation methods in colloid chemistry

Credits: 0 + 4

Coordinator/Department: Tibor Gilányi, Physical chemistry

Terms for joining: Basic knowledge in colloid and surface chemistry

Topics covered by the course:
Determination of the electrokinetic potencial by laser-Doppler electrophoretic measurements.
Dynamic light scattering measurements.
Wetting dynamics by tensiometric method.
Coagulation kinetiks by dead-stop method
Investigation of Langmuir films.
Determination of the electric charge of polyelectrolyte-surfactant complexes.
Dynamic surface tension by drop-profile analysis.
Investigation of interfaces by non-linear optical method (SFG).
Application of the atomic force microscope for the characterization of surfaces.

Literature*:
Compulsory: Notes on internet in progress
Suggested:
Wolfram Ervin: Kolloidika, Tankönyvkiadó, Budapest
R. J. Hunter: Foundation of Colloid Science, Clarendron Press, Oxford, 1993

Title of the course: Quantum mechanical foundation of structure determining methods

Credits: 2

Coordinator/Department: Attila G. Császár / Physical chemistry

Terms for joining: Basic knowledge in physics and theoretical chemistry

Topics covered by the course:
The purpose of the course is to acquaint the students, based on knowledge of physical chemistry gained earlier, with the methods of quantum chemistry and details concerning methods used for structure determination. Potential energy and property hypersurfaces; Hamilton operators based on the Coulomb interaction and beyond, their theory and application; practical methods to take relativistic effects into consideration, with emphasis on first- and second-order perturbation theory; theory of interaction of electromagnetic fields and matter; time-dependent perturbation theory; determination of vibrational levels with variational and perturbational techniques; the GF method; theory of electronic spectra; theory of NMR spectra.

Literature*:
Compulsory: Notes on internet in progress
Suggested:
Frank Jensen: Introduction to Computational Chemistry, Wiley, 1999.
Ira N. Levine: *Molecular Spectroscopy*, Wiley-Interscience: New York, 1975
Ira N. Levine: *Quantum Chemistry*, Wiley-Interscience: New York, 1999.

Title of the course: Reaction Kinetics

Credits: 3
Coordinator, Department:: Ernő Keszei, Physical Chemistry

Prerequisits: B.Sc. courses physical chemistry 1 and 2

Topics of the course:

Molecular theories of chemical reactions. Potential energy surfaces. Quasi-equilibrium and dynamic derivation of the Transition State Theory rate constant. Variational Transition State Theory. Classical and quantum-mechanical simulations to calculate rate constants. Analytical and numerical solutions of large reaction mechanisms. Reduction of the number of species and reactions. Quasi-steady-state approximation and its error. Reactions in liquid solutions. Ionic and polar transition states in polar solvents. Kinetic salt effects. Diffusion controlled reactions. Reaction-diffusion systems. Isotope effects. Linear free energy relationships and other semi-quantitative relations. Photochemistry. Radiation chemistry. Kinetics of enzyme-catalyzed reactions. Acido-base catalysis. Experimental methods in chemical kinetics. Molecular dynamics and laser photolysis experiments. Ultrafast lasers and femtochemistry. Exact quantum mechanical calculations of rate constants for reactions containing 3-4 atoms. Exotic dynamic systems; oscillations, pattern formation a chaos.

Textbooks to use

Compulsory: M.J. Pilling, P.W. Seakins: Reaction Kinetics, Oxford University Press, 1995
Recommended: P. W. Atkins: Physical Chemistry, Oxford University Press, 2005

Title of the course: Self- Organized Systems of Macromolecules and Biopolymers KV2KL3

Credits: 2 + 0

Coordinator/Department: Ferenc Csempesz, Physical Chemistry

Lecturer: Miklós Nagy

Terms for joining: Basic knowledge in physical and colloid chemistry

Topics covered by the course:
Composition and structural characteristics of macromolecules and polymers. Basic principles of polymer chemistry. Chemical and physical characterization of macromolecules. Conformation of synthetic and natural macromolecules. Properties of one and multicomponent macromolecular systems. Association phenomena: hierarchic and self-assembled structures. Ordering and organization. Relationships between structure and function. Experimental methods.

Literature*:

Compulsory:

Wolfram Ervin: Kolloidika, (lecture notes) egyetemi jegyzet I. - III. kötet, kijelölt fejezetek

Rohrsetzer Sándor: Kolloidika, (book) Tankönyvkiadó, kijelölt fejezetek

Suggested:

L. Mandelkern: An Introduction to Macromolecules English Univ. Press, London, Springer-Verlag, Berlin, New York, Heidelberg, 1972

H. Morawetz: Macromolecules in Solution, John Wiley and Sons, New York, London, Sydney, Toronto, 1975

A.G. Walton, J. Blackwell: Biopolymers, Academic Press, New York, London, 1973

Title of the course: Statistical Mechanics

Credits: 3+0

Coordinator/Department: András Baranyai, Physical chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:

The aim of statistical mechanics
Chaotic dynamics of molecules
Conservative and dissipative systems
Ergodic hypothesis and mixing
Microcanonical ensemble
Rationalization of the 2^{nd} axiom of thermodynamics
Canonical ensemble
Thermodynamic potential functions and other ensembles
Relations between the partition function and thermodynamic properties
Fluctuations and nonequilibrium systems
Theories of transport
Comparison with quantum statistical mechanics
Basics of gas, liquid and solid state statistical mechanics
Computer simulations as experiments

Literature*:
Compulsory: Lecture notes
Suggested: Baranyai A, Schiller Róbert, Statisztikus mechanika vegyészeknek ,Akadémiai, 2003.

Title of the course: Supplemental chapters to physical chemistry

Credits: 2+0

Coordinator/Department: András Baranyai, Physical chemistry

Terms for joining: Physical chemistry BSc

Topics covered by the course:
Chapters not or only superficially covered by the Physical Chemistry BSc courses 1-2. (e.g. Axiomatic thermodynamics, nonequilibrium thermodynamics and transport processes, thermodynamics for engineers, basics of hydrodynamics and rheology, introduction to solid state physics, liquid crystals, quasi-crystals, glasses, introduction to the theory of chaos and fractals, information theory.

Literature*:
Compulsory: Lecture notes
Suggested: Baranyai A, Schiller Róbert, Statisztikus mechanika vegyészeknek ,Akadémiai, 2003.

Title of the course: Physical Chemistry Laboratory (2)

Credits: 5

Coordinator/Department: Győző G. Láng, professor , Institute of Chemistry, Department of Physical Chemistry

Terms for joining: Basic knowledge in mathematics, physics and physical chemistry. Prerequisites are Physical chemistry(2) and Physical chemistry laboratory(1) or their equivalents.

Topics covered by the course:
This course is intended to acquaint the students with the practice of experimental physical chemistry. The goal of the labs is to gain familiarity with a variety of physicochemical measurement techniques. The development of high-level laboratory skills and the ability to use them in the reseach work are key aims of the course. The main topics are: Experimental study of phase and chemical equilibria using conductometry, spectrophotometry, and potentiometry. Determination of equilibrium constants. Experimental investigation of transport processes in chemical systems, determination of characteristic parameters. The dependence of viscosity on temperature. Measuring the viscosity with a falling ball (Höppler) viscosimeter. Fundamentals of Gas Chromatography. Study of the chemical kinetics of homogeneous and heterogeneous reactions. Determination of rate coefficients. Electrochemical measurements: mean activity coefficients from cell measurements, transport processes in electrolyte solutions, kinetics of electrode processes. Determination of pH and ion product for water. Study of electrochemical power sources.

Literature*:
Szalma, J., Láng, G., Péter, L.: Fundamental methods in the physical chemistry laboratory – measurements and data processing (English version in preparation)
Caria, M.: Measurement Analysis, Imperial College Press, London, 2000.
Garland, C.W., Nibler, J.W, Shoemaker, D.P.,: Experiments in Physical Chemistry, McGraw-Hill, New York, 2002.
Atkins, P.W.: Physical Chemistry, 7th edition, London, 1998

Optional specialized chemical courses

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Analytical Chemistry - specialized module

Title of the course: Analysis of Pharmaceutics

Credits: 2

Coordinator: Sándor Görög

Department: Richter Gedeon Rt.

Prerequisites: BSc level knowledge in analytical chemistry, chromatography and spectroscopy

Topics covered by the course:
Analysis of pharmaceutics, industrial applications emphasized.
Chemical analysis in pharmaceutical research and production.
Official organization of pharmaceutical analysis.
Analysis of raw materials and end-products. Effects of drugs in biological samples.
Selected topics: enantiomer-analysis, capillar electrophoresis

Literature:
Suggested books:
handouts and selected articles

Title of the course: Chemistry of Air

Credits: 2

Coordinator: Salma, Imre

Department: Department of Analytical Chemistry

Prerequisites: Environmental Chemistry or equivalent knowledge

Topics covered by the course:

- global climate, the role and importance of air constituents in the evolution and change of climate
- types, formation processes and dynamics of atmospheric aerosols
- thermodynamics of aerosol particles
- chemical characterization of aerosol particles
- fundamental toxicology of air pollutants
- environmental and health impacts of atmospheric aerosols
- measurement of aerosols: aerodynamic, electrodymanic, and optical methods

Literature*:
Compulsory:
Mészáros, E., 1997. Levegőkémia, Veszprémi Egyetemi Kiadó.Papp, S., 2002. Biogeokémia, Veszprémi Egyetemi Kiadó.
Suggested:

Wayne, R.P., 2000. Chemistry of atmospheres, 3rd ed., Oxford University Press
Warneck, P., 1999. Chemistry of the natural atmosphere, 2nd ed., Elsevier
Seinfeld, J.H., Pandis, S.N., 1998. Atmospheric Chemistry and Physics, Wiley
Finlayson-Pitts, B.J., Pitts, J.N., 1990. Atmospheric Chemistry: Fundamentals and Experimental Techniques, Wiley
Holton, J.R., Curry, J.A., Pyle, J.A. (eds.), 2003. Encyclopedia of Atmospheric Sciences, Vols. 1̃6, Academic Press

Title of the course: Cosmo-chemistry

Credits: 2

Coordinator: Lévay, Béla

Department: Deptartment of Analitical Chemistry

Prerequisites: All the basic knowlede in nuclear physics and nuclear chemistry necessary for the understanding of the topic are presented during the course.

Topics covered by the course: The main topic of the lecture is the explanation and interpretation of the special pattern of the observed average abundances of the nuclids in the Universe which shows several important features. The three main processes resulting in the formation of the chemical elements are discussed: the nucleogenesis in the big-bang, the nucleosynthesis during the stellar evolution, and the spallation processes in the interstellar medium. The standard big-bang model, the formation of galaxies and stars and the evolution of stars are also discussed at a level necessary to understand the above processes.

Literature*:
Compulsory: Copy of the slides used during the course.

Suggested: Vértes Attila: Magkémia I. Tankönyvkiadó, Budapest, egyetemi jegyzet; Kiss István-Vértes Attila: Magkémia, Akadémiai Kiadó, Budapest

Title of the course: Environmental Analytical Chemistry

Credits: 2

Coordinator: Záray, Gyula

Department: Department of Analytical Chemistry

Prerequisites: environmental chemistry, instrumental analytical chemistry

Topics covered by the course:

In-situ and laboratory techniques for determination of gaseous and solid pollut ants in the air from the sampling to the evaluation of analytical data. Analytical methods for determination of organic and inorganic pollutants in waste-, surface and drinking water. Passive and active monitoring of water quality; chemical and biological procedures.

Literature:

Compulsory:
Dinya-Suszter-Kiss-Papp-Bak: Környezetszennyező szerves vegyületek analitikája, Debreceni Egyetem, Jegyzet, 2002.
Ernő Mészáros, Levegőkémia, Veszprémi Egyetemi Kiadó, 1997.

Suggested:
Manahau S.E.: Environmental Chemistry, Lewis Publisher, 1994.
Cornelis-Caruso-Heumann: Handbook of Elemental Speciation II. Wiley, 2005.

Title of the course: Environmental Chemistry and Environmental Analysis Lab

Credit: 2

Coordinator: Orgoványi, Judit

Department: Department of Organic Chemistry

Prerequisites: admission to Chemistry Msc, basic knowledge in chemical technology and analytical chemistry

Topics covered by the course:

Measurement of hydrocarbon emission of petrol-driven vehicles using gas-chromatography.
Determination of nickel compounds in dust-ash of power-plants.
Measurements of electrokinetical potention using microelectrophoresis.
Waste water treatment with activated sludge in laboratory scale.
Determination of water contaminants using gas chromatography.
Applications of HPLC in environmental analytical chemistry.
Applications of inductive coupled plasma atomemission spectrometry in environmental analytical chemistry.
Dynamic wettability measurements.
Determination of corrosion rate by measuring polarization resistance.
Investigation of anodic passivation of metals using cyclic voltammetry.

Compulsory literature:
Dr. Varga Enikő, Garay Ferenc: Környezetkémiai analitika – környezettechnológiai praktikum, ELTE Eötvös Kiadó, Budapest
Instructions of measurements

Suggested literature:

Title of the course: Equilibrium Studies of Supramolecular Systems

Credits: 2

Coordinator: Buvári-Barcza, Ágnes

Department: Department of Analytical Chemistry

Prerequisites: basic knowledge of inorganic, organic and analytical chemistry

Topics covered by the course:

The formal (apparent) stability constants in supramolecular systems. Speciation - with examples.

Methods for the determination of stability constants (solubility, calorimetry, NMR, capillary electrophoresis, potentiometry, spectrophotometry) - their reliability and sources of uncertainties.

Some equilibria discussed in details: the interactions of some acid-base indicators with cyclodextrins; cyclodextrin complexes of inorganic ions, nitrophenols, organic acids and bases, C_{60} fullerene etc. Substituted cyclodextrins: the effect of the degree of substitiution (DS) and of the position of the substituents on the stability constants. Guest enforced solubility.

Literature*:

Compulsory:

Suggested:

M.T. Beck - I. Nagypál: Coordination Chemistry, John Wiley, Chichester, 1990

J. Szejtli and T. Osa (Eds.) Cyclodextrins. In: J.-M. Lehn, J.L. Atwood, J.E.D. Davies, D.D. MacNicol and F. Vögtle (Eds.): Comprehensive supramolecular chemistry, Vol. 3, Pergamon, Oxford 1989

V.T. D'Souza and K.B. Lipkovitz (Eds.): Cyclodextrins, Chemical Reviews, **98** (1998) 1741-2076 [http://pubs.acs.org]

Title of the course: Evaluation Methods of Analytical Chemistry Data

Credits: 2

Coordinator: Virág, István

Department: Department of Analytical Chemistry

Prerequisites: BSc level knowledge in Analytical Chemistry and Mathematics

Topics covered by the course:

Measurement error in analytical chemistry - error propagation
Error calculation (residual variance) – statistics – hypothesis testing
Correlation- and regression analysis
Nonlinear curve fitting – parameter estimation
Approximate calculus: differential and integral calculus
Application of modern computational methods for evaluation of the analytical chemistry results

Literature*:
Compulsory:

Suggested:

Veress Gábor, Pungor Ernő: Az analitikai kémiai adatfeldolgozás főbb módszerei, Tankönyvkiadó, Budapest, 1982

Szalma József: Mérési eredmények kiértékelésének alapjai, Tankönyvkiadó, Budapest, 1984

Title of the course: Gas-chromatography and High Pressure Liquid Chromatography

Credits: 2

Coordinator: Perl, Miklósné

Department: Department of Analytical Chemistry

Prerequisites: admission to Chemistry MSc, basic knowledge in analytical chemistry

Topics covered by the course:

History of chromatography, comparison of GC and HPLC: requirements, possibilities and results, analysis of hydroxyl group containing organics, analysis of carboxyl group containing organics, analysis of amino acids, simultaneous analysis of sugars, sugar alcohols, amino- and carboxylic acids, as well as flavonoids: identification/quantization of the composition of natural matrices

Literature:
Compulsory:

Suggested:

Title of the course: Harms and Protection of the Environment KV6KR2

Credits: 2

Coordinator/Department: Katalin Barkács assistant professor, Department of Analytical Chemistry

Terms for joining: basic terms of Chemistry MSc., basic chemical knowledge (Chemistry BSc., or either courses: KA6TC3, KV6KR1 - or equivalent knowledge)

Topics covered by the course:
Environmental management. Sources and removal of air-, water-, soil (gas-, liquid- and solid state) pollutants. Main environmental impacts of industrial-, agricultural-, communal- and traffic (transport) caused emissions, effects of noise and vibration. Qualification and handling of solid wastes, sludge and wastewaters. Life-cycle, recycling, handling, reuse and disposal of the different waste types. Economic-, legislated- and technical solutions, technology oriented basic strategies of pollution prevention and environmental protection.

Literature:
Compulsory:

Suggested:

http://www.kemtech.net, www.kvvm.hu,

Selected chapters of environmental protection handbooks, e.g.:

P.N.Cheremisinoff -Y.C.Wu: Hazardous Waste Management Handbook, Prentice-Hall Int. Limited, London (UK), 1994

J.C. Mycock, J.D. McKenna, L. Theodore: Handbook of Air pollution Control Engineering and Technology, Lewis Publishers, CRC Press Inc., New York (US), 1995

H.F.Lund: The McGraw-Hill Recycling Handbook, McGraw-Hill Inc., New York (US), 1993

Gy. Filep: Soil Chemistry, Akadémiai Kiadó, Budapest, Hungary, 1999

(in English)

Title of the course: Hyphenated Techniques for Element Speciation in Environmental Samples

Credits: 2

Coordinator: Mihucz, Viktor Gábor

Department: Department of Analytical Chemistry

Prerequisites: Admission to Chemistry MSc

Topics covered by the course: general characterization of off-line (HPLC-GF-AAS, HPLC-TXRF, TLC/OPLC-TXRF, TLC-LA-ICP-MS) and on-line techniques (HPLC-FAAS, HPLC-ICP-AES, HPLC-ICP-MS, GC-AAS, LC-QF-AAS) for element speciation in environmental chemistry; speciation of As, Cd, Cr, Hg, Ni, Pb and Sn in Environment.

Literature*:

Compulsory:

Az elemanalitika korszerű módszerei (Szerk.: Záray Gyula), Akadémiai Kiadó, 2006

Handbook of Elemental Speciation (Eds.: R. Kertulis, H. Crews, J. Caruso, K.G. Heumann), Wiley, 2005

Suggested:

Modern Methods for Trace Element Determination (Eds.: C. Vandecasteele and C.B. Block), Wiley, 1995

Practical HPLC method development (Eds.: L.R. Snyder, J.J. Kirkland, Glajch J.L.), Wiley, 1997

Atomic Absorption and Plasma Spectrometry (Ed.: J. R. Dean), Wiley, 1997

Students will receive the material of this course electronically in Reader Acrobat form.

Title of the course: Instrumental Nuclear Analytical Methods

Credits: 2

Coordinator: Salma, Imre

Department: Department of Analytical Chemistry

Prerquisites: basic knowledge in nuclear chemistry or physics

Topics covered by the course:

Place and role of nuclear analytical methods among the analytical methods: advantage, limits, and specialties

Instrumental neutron activation analysis (INAA):

- the principle and main steps of the method; kinetics of complex nuclear transformations (radioactive decay and nuclear reaction); the Bateman-Rubinson equation; activation neutron sources; γ-ray spectrometry: types, characteristics, and calibration of spectrometers; methods of INAA: absolute, relative, comparator, and parametric standardization; prompt-γINAA; environmental applications

Proton-induced X-ray Emission Spectrometry (PIXE)

- interaction of light charged particles with the matter; accelerators utilized for PIXE, and their properties; characteristic X-rays, energy disperse X-ray spectrometry; methods of PIXE: standardization for thick and thin targets; micro-PIXE; environmental applications

Literature:

Compulsory:
Salma, I., Műszeres neutronaktivációs analízis. In: Az elemanalitika korszerű módszerei, szerk. Záray, Gy., 417–505. old., Akadémiai Kiadó, Budapest, 2006.

Suggested:
Ehmann, W.D. – Vance, D. E.: Radiochemistry and Nuclear Methods of Analysis. Willey, New York 1991.
Erdtmann, G. – Petri, H.: Nuclear Activation Analysis: Fundamentals and Techniques. In: Treatise on Analytical Chemistry (Eds.: Elving, P. J. – Krivan, V. – Kolthoff, I. M.), Willey, New York 1986.
Vértes, A. – Nagy, S. – Klencsár, Z. (Eds.): Handbook of Nuclear Chemistry. Kluwer Academic Publishers, Dordrecht 2003.

Title of the course: Introduction into Nuclear Environmental Protection

Credits: 2

Coordinator: Homonnay, Zoltán

Department: Department of Analytical Chemistry

Prerequisites: admission to Chemistry MSc, basic knowledge in physics and chemistry

Topics covered by the course:
Interaction between radiation and matter. Dose concepts, principles of dosimetry and types of dosimeters. Biological effects of radiation. Basic principles of radiation protection. Determination of internal and external dose. Sources of natural and artifical radiation dose. The nuclear fuel cycle and the operation principles of nuclear reactors. Dynamic behavior of nuclear reactors, the problems of controlling the chain reaction, nuclear accidents. Nuclear waste storage and disposal. Safety of the nuclear energy production, trends in inceasing safety and solving nuclear waste problem in the future. Methods and current practice in nuclear environmental control.

Literature*:

Compulsory:

Attila Vértes, István Kiss: Nuclear Chemistry, *Akadémiai Kiadó,* Budapest, 1987

Suggested:

Attila Vértes, Sándor Nagy, Zoltán Klencsár: Handbook of Nuclear Chemistry, Kluwer, Amsterdam, 2003
Joseph Magill, Jean Galy: Radioactivity, Radionuclides, Radiation, Springer, Berlin, 2005
G. Choppin, J.O.Liljenzin, J.Rydberg, Radiochemistry and Nuclear Chemistry, Butterworth-Heinemann, 2002.

Title of the course: Investigation Methods of Material Structures, Lab

Credits: 6

Coordinator: Sinkó, Katalin

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in instrumental analytical and physical chemistry

Topics covered by the course:
FT IR – RAMAN spectroscopy; Mössbauer spectroscopy, Positron annihilation; MAS NMR spectroscopy; Electrochemical corrosion; CDV technique; Electron microscopy; AFM ;Neutron diffraction and scattering; X-ray scattering; Ellipsometry

Literature:

P. Lindner, Th. Zemb (eds): Neutron, X-Ray and Light Scattering, North-Hollnad, Oxford, 1991.

Title of the course: ISO 9000 and Analytical Chemistry

Credits: 2

Coordinator: Varga, Imre

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in analytical chemistry

Topics covered by the course:
History of quality assurance, definitions used in standards of ISO 9000 group, quality control and assurance in analytical laboratory, examples from industrial and research laboratories.

Literature:
Suggested books:

Title of the course: Microanalytical Measurement Techniques

Credits: 2

Coordinator: Varga, Imre

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in analytical chemistry

Topics covered by the course:
Fundamentals of emission and absorption spectra of atoms, atom and ion sources used in microanalysis, characteristics of X-ray fluorescence, total-reflection and its consequences, detection of ions from an ICP by mass spectrometry, comparison of analytical features of selected methods.

Literature:
Suggested books:

Title of the course: Modern Electroanalytical Methods

Credits: 2

Coordinator: Inzelt, György

Department: Department of Physical Chemistry

Prerequisites: BSc degree, basic knowledge in analytical chemistry and electrochemistry

Topics covered by the course: Ionselective electrodes, potentiometry, determination of pH. Sensors, biosensors.Voltammetric techniques: cyclic voltammetry, pulse voltammetries, square-wave voltammetry, stripping voltammetry. Ac techniques. Electroanalysis of solid materials. Spectroelectrochemical methods. Microelectrodes.Electrochemical nanogravimetry

Literature:

Compulsory: **Electroanalytical Methods, F.Scholz (ed), Springer, Berlin, Heidelberg, 2002;**
A.J.Bard, L.R.Faulkner: Electrochemical Methods, Wiley, 2001.

Suggested:
Electroanalytical Chemistry. A series of Advances, Vols 1-22, Marcel Dekker,
G.Harsányi: Polymer Films in Sensor Applications, Technomic, Lancester,Basel, 1995;
C.M.A. Brett, A.M.Oliveira-Brett: Electrochemistry, Principles, Methods and Applications, Oxford Univ.Press, Oxford, 1993; Microelectrodes (eds.: M.I.Montenegro, M.A. Queirós,J.L.Daschbach) , Kluwer,1990.

Title of the course: Modern Instrumental Methods in Analytical Chemistry

Credits: 8

Coordinator: Tatár, Enikő

Department: Department of Analytical Chemistry

Prerequisites: BSc level knowledge in analytical chemistry

Topics covered by the course:
Transmission electronmicroscopy, gas chromatography / mass spectrometry, ion chromatography, electrophoresis, ultra micro electrodes, scanning electronmicroscopy, electron beam micro-analysis

Literature:
Compulsory:
handouts

Suggested books:
selected articles

Title of the course: Monitoring Methods for the Quality of Water

Credits: 2

Coordinator: Óvári, Mihály

Department: Department of Organic Chemistry

Prerequisites: Analytical Chemistry and Environmental Chemistry from Chemistry BSc or equivalent knowledge

Topics covered by the course:
Surface waters and their characterisation. The water quality and its parts. Biological and chemical qualification. Methods of sampling, sample preparation, analysis, statistical evaluation of results. Practical examples.

Literature:
Záray Gy. (Ed.): Az elemanalitika korszerű módszerei, Akadémiai, 2006.
Felföldy L.: A biológiai vízminősítés. 4. kiad. In: Vízügyi Hidrobiológia 16. VGI, Budapest, 1987.
Dévai Gy. (Ed.): Vízminőség és ökológiai vízminősítés. Acta biol. debrecina, Suppl. oecol. hung. 4, 1992
Dévai Gy., Végvári P., Nagy S., Bancsi I. (Eds.): Az ökológiai vízminősítés elmélete és gyakorlata. 1. rész. – Acta biol. debrecina, Suppl. oecol. hung. 10/1, 1999.
Water Guideline - 2000/60/EK Guideline. – English-Hungarian, Version of Feb 24, 2002. BMKE, Budapest.

Title of the course: Mössbauer Spectroscopy: Principles and Applications

Credits: 2

Coordinator: Kuzmann, Ernő

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in nuclear chemistry or nuclear physics

Topics covered by the course:
Principles of Mössbauer spectroscopy. Hyperfine interactions. Characterization of Mössbauer spectra. Mössbauer parameters. Measurement techniques. Spectrum evaluation. Applications. Analytical information from Mössbauer spectra. Qualitative and quantitative analytical applications. Chemical applications. Biochemical applications. Applications in nuclear physics. Solid state physical applications. Industrial applications. Another applications.

Literature:
Suggested books:
N.N. Greenwood, T. C. Gibb, Mössbauer Spectroscopy, *Chapman and Hall*, London ,1971
U. Gonser (Ed): Mössbauer Spectroscopy, Topics in Applied Physics, *Springer*, Berlin, 1975.
A. Vértes, L. Korecz, K. Burger: Mössbauer Spectroscopy, *Elsevier*, Amsterdam, 1979.
E. Kuzmann, Z. Homonnay, S. Nagy, K. Nomura: Mössbauer spectroscopy, in Handbook of Nuclear Chemistry (Eds. Vértes A., Nagy, S., Klencsár, Z.) Kluver, Vol. 3.

Title of the course: New Chemical Methods in Material Science A

Credits: 2

Coordinator: Sinkó, Katalin

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in inorganic and colloid chemistry

Topics covered by the course:
Preparation of precursors: organic, inorganic, and metalorganic starting materials (Special gases; metals, alloys; covalent and ionic hydrides; metal halogenides, -oxides, -sulfides; -alkoxides, -carboxilates; metal complexes; precursors of ceramics); New preparation routes of amorphous systems, sol-gel technique (chemical processes of sol-gel method: hydrolysis, condensation, drying gel systems, heat treatment, advantages and disadvantages of sol-gel methods, industrial applications); Polymer gels, chemical and structural modifying methods (physical and chemical properties of polymers, functional polymers, polymer based nanostructures, nanohybrides); Non-conventional materilas and theirs properties: medical, biotechnological and automata technical applications (artificial muscles, drug delivery systems), elektrostrictive, magnetostrictive and piezoelectric materials, elektroreological, magnetoreological and magnetic liquids, shape-memory metal and polymers)

Literature:
Brinker, C. J.; Scherer, G. W. *Sol-gel Science*; Academic Press: Boston, 1990.
R. W. Cahn: The coming of materials science, Pergamon, Amsterdam,
W. D. Callister: Materials Science and Engineering, An Introduction, Wiley,
W.F. Smith: Principles of Materials Science and Engineering, McGraw-Hill Publ.

Suggested books:
J. Frommer, R.M. Overney, Interfacial Properties on the Submicrometer Scale, Am. Chem. Soc., Washington, 2000.
C.N.R. Rao, A. Müller, A.K. Cheetham, The Chemistry of Nanomaterials, Wiley-VCH Verlag, Weinheim, 2004.

Title of the course: Nuclear Methods with Applications in Biology

Credits: 2

Coordinator: Homonnay, Zoltán

Department: Department of Analytical Chemistry

Prerequisites: admission to Chemistry MSc, basic knowledge in physics and chemistry

Topics covered by the course:
Review of the basics of nuclear chemistry, application of radiation for diagnostic purpose and for its radiation effect. Nuclear techniques in biology: isotope dilution, radioimmunoassay, radiotracer techniques in plant and animal physiology as well as in human application. Preparation and application of isotopically labelled compounds, PET-diagnostics, CT and other imaging techniqes. Radiotherapy, nuclear medicine, biological consequences of radiation exposure. The basics of stable isotope labeling and applications in analytical chemistry; isotope effects.

Literature:
Compulsory:
Attila Vértes, István Kiss: Nuclear Chemistry, *Akadémiai Kiadó,* Budapest, 1987

Suggested:
Handbook of Nuclear Chemistry, ed. A. Vértes, S. Nagy, Z. Klencsár, Kluwer Academic Publishers, 2003 relevant chapters
Joseph Magill, Jean Galy: Radioactivity, Radionuclides, Radiation, Springer, Berlin, 2005
G. Choppin, J.O.Liljenzin, J.Rydberg, Radiochemistry and Nuclear Chemistry, Butterworth-Heinemann, 2002.

Title of the course: Nuclear investigating methods

Credits: 3

Coordinator: KUZMANN, Ernő

Department: Department of Analytical Chemistry

Prerequisites: Basic knowledge in nuclear chemistry or nuclear physics

Topics covered by the course:
Nuclear methods for analytical purpose. Röntgenfluorescence analysis with radioactive sources. Methods based on absorption and scattering of nuclear radiations. Activation analysis and its application. Rutherford backscattering method. Nuclear methods in structural chemistry. Basic (hyperfine interactions, Mössbauer parameters) techniques and applications of Mössbauer spectroscopy. Basic of positron annihilation spectroscopy. Neutron spectroscopy, neutron diffraction (neutron sources, basics of neutron spectroscopy, polarization of neutrons, neutron spin echo, neutron diffraction) and applications. Nuclear magnetic resonance (basics of NMR, relaxation times and their measurement methods) and metal physical applications. Nuclear power plants. Accelerators (Cocroft-Walton accelerator, cyclotrons). Ion implantation and its applications. Radioactive trace methods and their analytical applications in technological processes. Industrial applications. Industrial radiography.

Literature:
Suggested books:
Dezsõ Kiss and Zsolt Kajcsos, Nuclear Technics, Tankönyvkiadó, Budapest, 1984.(in Hungarian)

Title of the course: Nuclear investigating methods laboratory

Credits: 2

Coordinator: KUZMANN, Ernő

Department: Department of Analytical Chemistry

Prerequisites: Basic knowledge in nuclear chemistry or nuclear physics. The course is linked to the lecture entitled Nuclear investigating methods

Topics covered by the course:
Instrumental laboratory practice. Radioactive source induced Röntgenfluorescence analysis. Mössbauer spectroscopy. Reactor techniques. Nuclear magnetic resonance. Positron annihilation spectroscopy. Liquid scintillation. Prompt gamma analysis. Neutron activation analysis.

Literature:
Notes for the measurements
Suggested books:
Dezsõ Kiss and Zsolt Kajcsos, Nuclear Technics, Tankönyvkiadó, Budapest, 1984.(in Hungarian)

Title of the course: Nuclear Techniques in Structural Chemistry

Credits: *2*

Coordinator/Department: ***Attila Vértes/Department of Analytical Chemistry***

Terms for joining: ***Basic knowledge in mathematics, physics and chemistry.***

Topics covered by the course:

- Physical background of Mössbauer spectroscopy (MS).
  Experimental techniques of the transmission, reflection and conversion electron MS.
  Mössbauer measurements with synchrotron radiation.
- Theoretical aspects of positron annihilation spectroscopy (PAS).
  The methods of angular correlation (ACS), Doppler broadening (DBS) and positron- and postironium-lifetime spectroscopies (PLS)
- Description of the phenomena of muon spin-relaxation, -rotation, and – resonance (μSR) and their applications for structural studies.
  The formation of heavy exotic atoms and their interactions with matter as a probe for material science.
- Several applications of the discussed techniques in structural chemistry and material science.

Literature*:

Compulsory:

A. Vértes, I. Kiss: Nuclear Chemistry, Akadémiai Kiadó, Elsevier, 1987.

A. Vértes, L. Korecz, K. Burger: Mössbauer Spectroscopy, Akadémiai Kiadó, Elsevier, 1979.

Suggested books:

A. Vértes, S. Nagy, Z. Klencsár (editors): Handbook of Nuclear Chemistry, Kluwer Academic Publishers, 2003.

Title of the course: Plasma spectroscopy

Credits: 2

Coordinator: Záray, Gyula

Department: Department of Analytical Chemistry

Prerequisites: environmental chemistry, instrumental analytical chemistry

Topics covered by the course:

General characterization of AC and DC arc, spark and glow discharges, as well as “high frequency” plasmas working in the MHz-GHz range (inductively coupled and microwave induced plasma). Sample introduction into the plasma sources. Comparison of analytical capabilities (detection limits, reproducibility, dynamic range, sensitivity etc.) of different plasma sources and demonstration of their applicability in different fields of analytical chemistry.

Literature:
Compulsory:

Az elemanalitika korszerű módszerei, Edited by Záray Gyula, Akadémiai Kiadó, 2006.

Suggested:
Glow Discharge Plasmas in Analytical Spectroscopy, Edited by R.K.Marcus and J.A.C. Broekaert, Wiley, 2003.
Inductively Coupled Plasmas in Analytical Atomic Spectrometry, Edited by A. Montaser and D.W. Golightly, 1987.

Title of the course: Preconcentration Methods in Atomic Spectrometry

Credits: 2

Coordinator: Zihné Perényi, Katalin

Department: Department of Analytical Chemistry

Prerequisites: Instrumental Analysis I. or equivalent knowledge and practice, basic knowledge of atomic spectrometric techniques

Topics covered by the course:
Definitions. Control of contamination and loss. Flow injection analysis,(FIA). Hydride generation. Liquid-liquid extraction. Precipitation and coprecipitation. Sorbens extraction: Sorption of metal-chelates on nonpolar sorbents and retention of metal ions by chelating agent adsorbed on a support. Enrichment by ion-exchange, chelating exchange. Hyphenated techniques: Join separation techniques (HPLC, GC, capillary GC, capillary electrophoresis – CE) with Atomspectrometric detectors (ICP-AES, ICP-MS, GFAAS, FAAS etc.). Field flow fractionation (FFF): separation and preconcentration

Literature*:
Compulsory:
The slides of the lecture are available for the students in electronic form.

A. Mizuike: Enrichment Techniques for Inorganic Trace Analysis, Springer-Verlag, Berlin-Heidelberg-New York, 1983

Suggested:

Z. Fang: Flow Injection Atomic Absorption Spectrometry, Wiley, 1995
F. Macásek, J.D. Navratil: Separation Chemistry, Ellis Horwood, New York, London, 1992
Flow Injection Atomic Spectroscopy, ed. by J.L. Burguera, Marcell Dekker Inc., New York, Basel, 1989

Title of the course: Radiation Protection

Credits: 2

Coordinator: Homonnay, Zoltán

Department: Department of Analytical Chemistry

Lecturer: Fehér, István

Prerequisites: admission to Chemistry MSc, basic knowledge in nuclear chemistry (e.g., Basics of Nuclear Chemistry in BSc, Chemistry, ELTE, KA2MG1)

Topics covered by the course:
Purpose and subject of radiation protection. Dose concepts. Hazardous effect of ionizing radiation on humans. Natural and artifical sources of dose on large populations. Basic principles of radiation protection according to the guidlines of ICRP-60 and IBSS. Methods of dosimetry in controlling the dose of personnel. Methods in controling radio-emission into natural waters and the atmosphere. Principles of protection against sealed and open radioactice sources. Internal dose. Classification of nuclear waste and waste disposal. Main methods of nuclear environmental control. Law on the application of nuclear energy in Hungary (1996. CXVI.). Ministerial Decree on the rules and regulations in radiation protection in Hungary (16/2000 /VI.8, EüM).

Literature*:
Compulsory:
Attila Vértes, István Kiss: Nuclear Chemistry, *Akadémiai Kiadó,* Budapest, 1987

Suggested:
Handbook of Nuclear Chemistry, ed. A. Vértes, S. Nagy, Z. Klencsár, Kluwer Academic Publishers, 2003 relevant chapters
Joseph Magill, Jean Galy: Radioactivity, Radionuclides, Radiation, Springer, Berlin, 2005
G. Choppin, J.O.Liljenzin, J.Rydberg, Radiochemistry and Nuclear Chemistry, Butterworth-Heinemann, 2002.

Title of the course: Radioanalytical Chemistry Lab

Credits: 4

Coordinator: Süvegh, Károly

Department: Deptartment of Analitical Chemistry

Prerequisites: admission to Chemistry MSc, basic knowledge in nuclear chemistry (for those having an ELTE Chemistry BSc: Basics of Nuclear Chemistry, KA2MG1; for others: equivalent knowledge)

Topics covered by the course:
The course is a laboratory practice covering the following topics: work with open radioactive sources; tracer techniques; isotope separation; X-ray fluorescence (XRF), gamma-spectroscopy; neutron activation analysis; promt-gamma spectroscopy; study of material structur with nuclear methods; dosimetry, radiation protection; environmental samples; environment protection.

Literature:
Compulsory:
Sylabus for the measurements (provided by the course, also in electronic form)
Kiss István, Vértes Attila: Magkémia I., Tankönyvkiadó, Budapest, 1975
Fodorné Csányi Piroska, Vértes Attila: Magkémiai gyakorlatok, *Tankönyvkiadó*, Budapest, 1990
Suggested:
Nagy Sándor: Nukleáris mérések statisztikája (Valószínűség-számítási összefoglaló alkalmazásokkal).
Books given in the Syllabus

Title of the course: Sampling and Sample Preparation Methods in Analitical Chemistry

Credits: 2

Coordinator: Tatár, Enikő

Department: Department of Analytical Chemistry

Prerequisites: admission to Chemistry Msc

Topics covered by the course:
The types of the samples; Sampling of gas, liquid and solid state materials, metals. Sampling for speciation analysis and for the analysis of environmental samples (air, waters, biological samples sediments and soils); Error sources of the sample preparation. Classic sample preparation methods (dissolving, decomposing, acidic flux, decomposition of organic compounds). Modern digestion methods (high temperature digestion with conventional heat transmission, microwave assisted digestion methods, dry ashing for decomposing organic (biological) samples. Aqueous reagents for dissolving or decomposing samples; Enrichment and separation methods; Sample preparation methods for speciation analysis

Literature:
Compulsory:
Záray Gy.: Az elemanalitika korszerű módszerei, Akadémia Kiadó 2006

Suggested:
R. Bock A Handbook of Decomposition Methods in Analytical Chemistry, Marr, I. L., 1st ed.; John Wiley and Sons: New York, 1979
H.M. Kingston, L.B. Jassie: Introduction to microwave Sample Preparation, ACS, Washington, DC, 1988
C. Vandecasteele and C.B. Block: Modern methods for trace element determination, John Wiley & Sons, Chichester, 1993
R.M. Reeve: Environmental Analysis, John Wiley & Sons, Chichester, 1994
D.A. Skoog, D.M. West, F.J. Holler: Analytical chemistry, Saunders College Publishing, Fort Worth, 1992

Title of the course: Selected Methods of Analytical Chemistry

Credits: 4

Coordinator: Záray, Gyula

Department: Department of Analytical Chemistry

Prerequisites: BSc level knowledge in analytical chemistry

Topics covered by the course:
Instrumental methods in modern analytical chemistry: analysis of environmental, food, cryminal, and pharmaceutical samples

Literature:
Compulsory:
Az elemanalitika korszerű módszerei, Szerk.: Záray Gyula, Akadémiai Kiadó, 2006
Applied Spectroscopy, Eds: J. Workman, A. Springsteen, Acadmic Press, 1998
Handbook of Environmental Speciation I: Techniques and Methodology, Eds.: R. Cornelis, J. Caruso, H. Crews, K. Heumann, Wiley, 2005

Suggested books:
Umweltanalytik und Ökotoxikologie, Eds.: S. Holler, C. Schaefers, J. Sonnenberg, Springer, 1996
Fernmessung von Luftverunreinigungen, Ed.: V. Klein, Ch. Werner, Springer-Verlag, 1993

Title of the course:	Soil and environment

Credits:	2
Coordinator/Department:	Sándor Papp, Department of Environmental and Landscape Geography, ELTE
Terms for joining:	Admission criteria for MSc

Topics covered by the course:

Natural and anthropogenic factors and preparatory processes of soil formation: fragmentation and weathering of rocks. Formation and types of clay minerals. Organic materials of soils and their role in soil formation. Development of soils; soil processes and their association. Genetic and soil geographical classification of soils in Hungary. Forming conditions and processes of the soil types.
Root causes and affecting factors of water and wind erosion. Dynamics of erosion of prevailing soil types and questions of their protection.
Impacts of anthropogenic activity on soils (formation of surface, cultivation, fertilizing, weed control, irrigation, amelioration etc.). Conditions of the formation of acid and alkaline soils, their physical, chemical and biological properties, methods and proceedings of their improvements.

Compulsory literature*:

Stefanovits P. et al. 1977. Talajvédelem, környezetvédelem. – Mezőgazdasági Könyvkiadó, Budapest.
Stefanovits P.–Filep Gy.–Füleky Gy. 1999. Talajtan. – Mezőgazda Kiadó, Budapest.

Suggested literature:

Papp S. 2003. A talaj mint megújuló és mint megújítható erőforrás. A földhasználat. – In: Bora Gy.–Korompai A. (szerk.): A természeti erőforrások gazdaságtana és földrajza (2., javított kiadás). – Aula Kiadó, Budapest. pp. 222–259.

* Együtt 3-5 könyv, jegyzet.

Title of the course: Solution Equilibrium Measurements, their Evaluation and Speciation Calculations

Credits: 2

Coordinator: Szakács, Zoltán

Department: Deptartment of Analytical Chemistry

Prerequisites: admission to Chemistry MSc, basic knowledge in analytical and physical chemistry, basic skills as a computer user

Topics covered by the course:

Study of protonation, metal ion and supramolecular complex formation equilibria by potentiometric, voltammetric, electrophoretic and spectrometric (UV, CD, NMR) techniques. Computer simulation, design and evaluation of direct or competitive titrations (interactive, ”hands-on” education in a computer room). Study of site-specific protonation and complexation: microspeciation, cooperativity of binding sites. Speciation calculations in the presence of several metal ions and ligands: competition, models of oceans and biological fluids.

Literature*:

Compulsory:

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Recommended:

Beck M. T., Nagypál I. *Chemistry of complex equilibria*.
Ellis Horwood Ltd., Chichester, 1990. (az előző kibővített kiadása angolul)

Martell A. E., Moteatikis R. J. *The determination and use of stability constants.*
VCH, New York, 1988.

Meloun M., Havel J., Högfeldt E. *Computation of solution equilibra*.
Ellis Horwood, Chichester, 1988.

Title of the course: Supramolecular Chemistry and Molecular Recognition

Credits: 2

Coordinator: Buvári-Barcza, Ágnes

Department: Department of Analytical Chemistry

Lecturer: Barcza, Lajos

Prerequisits: basic knowledge in inorganic and analytical chemistry

Topics covered by the course:

The molecular recognition is the first step of every biological processes included active transport, enzymatic synthesis or gene regulation, and plays an important role in separation techniques.

The lecture will deal with the theoretical backgrounds, with the principal interacions governing self-organization: (i) hydrogen bonding, (ii) electrostatic attraction, (iii) π-stacking and (iv) van der Waals attraction.

Based on this background, the main trends and models of present researches will be summarized, like drug design, artificial receptors, etc., together with the kinds of the most interesting hosts, like crown ethers, cryptands, hemispherands, spherands, macrocycles containing nitrogen, cyclodextrins, cyclophanes calixarenes, cavitands, carcerands etc.

Further topics are: characterization of the strength of the interacions; the role of supramolecular chemistry in analytical procedures.

Literature*:

Compulsory:

J.-M. Lehn: Supramolecular chemistry: from complexes to complexity

Angew. Chem. Int. Ed. Engl., **67** (1988) 89

Suggested:

D. J. Cram - J. M. Cram: Container molecules and their guests, The Royal Society of

Chemistry, 1994

G. Gokel: Crown ethers and cryptands, The Royal Society of Chemistry, 1991

Title of the course: Synchrotron and neutron radiation in chemical research

Credits: 2

Coordinator: Vankó, György

Department: outsider;)) -- Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in physics and nuclear sciences

Topics covered by the course:
Synchrotron radiation: production and properties. Basics of X-ray optics. Spectroscopic and diffraction techniques with high flux X-ray beams.
Neutron sources, properties of neutron beams, interactions of neutron with matter. Basics of neutron optics, detection of neutrons. Neutron scattering. Chemical analysis based on neutron activation analysis.

Literature:
Handouts, selected scientific papers.

Inorganic Chemistry - specialized module

Title of the course: Applied catalysis

Credit: 2

Coordinator /Department: András Kotschy associate professor, Department of Inorganic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in inorganic, organic and organometallic chemistry (successful exams in inorganic and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Fundamentals of organometallic chemistry, fundamentals of catalysis, olefin hydrogenation, asymmetric hydrogenation, hydroformilation, hydroamination, aminocarbonylation, alkoxycarbonylation, decarbonylation, cross-coupling reactions, reactions of allyl complexes, metathesis.

Compulsory literature*:
Faigl F., Kollár L., Kotschy A., Szepes L. Szerves fémvegyületek kémiája, *Nemzeti Tankönyvkiadó*, Budapest, 2001

Suggested literature:
A. Kotschy, G. Timári, Heterocycles from Transition Metal Catalysis, *Springer*, 2005

Title of the course: Astrochemistry

Credits: 2

Coordinator/Department: György Tarczay, Inorganic Chemistry

Terms for joining:

Topics covered by the course:

1. Introduction to Astronomy. Evolution and structure of the Universe. Big bang, nucleosynthesis. Abundance of the chemical elements.
2. A Basics of astronomical spectroscopy. Adsorption, emission, stimulated emission. Light sources. Optical density, critical density. Doppler-shift. Distance determination in astronomy. Astronomical masers and lasers.
3. Recording of astronomical spectra. Spectral windows of the atmosphere. Radio, IR, UV-VIS and X-ray telescopes. Spatial and spectral resolution. Ground based and satellite observations. (ISO, IRAS, Hubble, ….)
4. Evaluation of astronomical spectra. Laboratory experiments for preparation and spectral characterization of astronomical molecules and reactions. Theoretical calculations and their accuracy.
5. Interstellar Medium (ISM). Types and phases of ISM. Molecules observed in ISMs. Physical and chemical processes, kinetic models. Photochemical, ionic and grain-surface processes. Laboratory experiments (e.g. CRESU).
6. Star formation and stellar evolution. Relevant chemical processes.
7. Formation of the Solar System. Geochemical evolution of Earth. Evolution of the atmosphere. Atmospherical processes and their spectroscopical observation. (e.g. ACE: Atmospheric Chemistry Experiment).
8. Chemistry of comets and meteorites.
9. Chemistry of Mars, Venus, Jupiter and the larger satellites (Moon, Io, Europe, Titan). Missions.
10. Astrobiology.

Literature*:
Compulsory: -

Suggested: J. Tennyson: Astronomical Spectroscopy (Imperial College Press, 2005.)
T. W. HartQuist, D. A. Williams: The Chemically Controlled Cosmos (Cambridge University Press, 1992.)
A. M. Shaw: Astrochemistry, From Astronomy to Astrobiology (Wiley, 2006.)
Chemical Evolution of the Universe, Faraday Discuss. 2006.
A. G. G. M. Tielens: The Physics and Chemistry of Interstellar Medium
E. Herbst: The Chemistry of Interstellar Space, Chem. Soc. Rev. 2001, 30, 168-176.

Title of the course: Complex synthesis lab

Credit: 8

Coordinator /Department: Antal Csámpai associate professor, Department of Inorganic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exam in organic chemistry and passing of organic chemistry lab, for others: equivalent knowledge)

Topics covered by the course:

the completion of multi step syntheses (literature search, synthesis planning, isolation of intermediates, purification of intermediates, isolation of product, purification of product, structure verification)

Compulsory literature*:

Suggested literature:

Title of the course: Derivatization in chromatography

Credits: 2

Coordinator/Department: Mária Mörtl assistant professor, Department of Inorganic Chemistry

Terms for joining: for graduated students (MSc level) after Separation technics lecture and laboratory practice (ELTE BSc KV5LV1 and KV5LV2), or other equivalent studies on chromatographic methods

Topics covered by the course:
Problems in gas and liquid chromatography, which can be solved by derivatization (e.g. improve peak shape, separation and volatility), detector-oriented derivatives for ECD, MSD, etc., and derivatization reactions for different types of compounds, detailed treatment of silylation (silylating agents, stability of Si–O bond, mechanism of silylation), chiral derivatizations, techniques for derivatization (pre-, on and post column, etc.), practical examples (e.g. steroids, drugs, aflatoxins), some related fields, like cyclodextrines in capillar electrophoresis, surface modifications by silylation, etc.

Literature*:
Compulsory:
C. F. Poole, S. K. Poole: Chromatography today, Elsevier, Amsterdam, 1991, 848-914 o.
Lecture slides will be achieved electronically

Suggested:
Pierce Chromatography Catalog and Handbook, Rockford, 2003, www.piercenet.com
D. R. Knapp: Handbook of Analytical Derivatization Reactions, John Wiley and Sons, 1979
http://www.registech.com/chromatography
http://probes.invitrogen.com/handbook

Title of the course: Experimental Methods in Materials Science

Credits: 6

Coordinator: Homonnay, Zoltán

Department: Department of Analytical Chemistry

Prerequisits: admission to Chemistry MSc

Topics covered by the course: The aim of this laboratory practice course in the first half of the term is to offer a general overview to the students about modern preparation techniques in materials science, while in the second half, more detailed studies can be carried out in one particular field selected by the student. These techniques involve preparation procedures applied in solid state chemistry, colloid chemistry, electrochemistry, and other fields. For example, preparation of functional nanolayers by self-ordering, chemical surface modification, and Langmuir-Blodgett method, as well as synthesis of multicomponent disperse colloid systems, nanogels and aerogels are scheduled.

Literature*:
Compulsory: Lab manuals will be distributed for each technique and lab task.

Suggested: Books and science articles recommended by the teacher of the lab.

Title of the course: Homogeneous catalysis

Credits: 2

Coordinator: Simándi, László

Department: Department of Analytical Chemistry

Prerequisites: admission to Chemistry MSc, basic knowledge in inorganic chemistry and metal-organic chemistry

Topics covered by the course:
Types of metal-organic reactions, mechanisms of homgeneous catalitic reactions: reactions of olefins and hydrocarbons, reactions of carbon monoxide, enantio-selective reactions.

Literature*:
Compulsory:
Simándi László: Homogén katalízis (handout)
Suggested books:
selected articles

Title of the course: Introduction to organosilicon chemistry

Credits: 2

Coordinator/Department: Roland Szalay assistant professor/Department of Inorganic Chemistry

Terms for joining: inorganic chemistry, organic chemistry

Topics covered by the course:
Introduction of the Si atom into organic compounds and its influence on the physical and chemical properties thereof. The nature of the silicon-carbon and silicon-heteroatom bonds. General methods for the preparation of organosilicon compounds. The structure and reactivity of the main groups of organosilicon compounds. Preparation, structure investigation and characteristic reactions of reactive silicon compounds (silylenes and their derivatives). The chemistry of poly-silanes and -carbasilanes. The importance of the silicon substituted organic compounds in organic syntheses: the silyl group as blocking or activating group. Chemo-, regio- and stereoselective silylation methods. The use of organosilicon compounds in materials sciences, the importance of silsesquioxanes. Introduction to the bioorganosilicon chemistry, sila drugs.

Literature*:
Compulsory:
Greenwood - Earnshaw: Chemistry of the elements (Pergamon Press, 1989)
Elschenbroich – Salzer: Organometallics (Verlag Chemie, 1992)
Suggested:
The Chemistry of Organic Silicon Compounds (eds Z. Rappoport, Y. Apeloig, John Wiley & Sons, 2001)
Comprehensive Organometallic Chemistry II: Silicon Group, Arsenic, Antimony and Bismuth (ed. A.G. Davies, Pergamon, 1995)
Auner – Weis: Organosilicon Chemistry 5- From Molecules to Materials (John Wiley & Sons, 2003)

Title of the course: Laboratory Praxis in NMR and Mass Spectroscopy and X-ray Diffraction

Credits: 6

Coordinator/Department: Dr. János Rohonczy / Department of Inorganic Chemistry

Terms for joining: Fulfilement of courses "Modern Structural Research Methods" and "Laboratory Praxis of Modern Structural Research Methods"

Topics covered by the course:
The aim of this course is the detailed study of experimental aspects of NMR spectroscopy, mass spectrometry and X-ray diffraction techniques including the required data acquisition, processing steps and required computer software. At the end of this cource the sudent wiil be able to plan, perform experiments as well as to treat and evaluate the aquired data on his/her own. The topics of this course covers the most important 1D and 2D, homo- and heteronuclear NMR experiments both in solutions and solid phase (DEPT, COSY, HSQC, HMBC, CPMAS, etc.). The aim of the X-ray diffraction exercises is the introduction to the practical steps of the structure determination of the small molecular and protein crystals, the visualization of molecules and the handling of international crystallographic databases.

Literature*:
Compulsory:

Suggested:

P.J. Hore: Nuclear Magnetic Resonance, Oxford University Press, 1995. (ISBN13: 9780198556824, ISBN10: 0198556829)
Rohonczy János: Szilárd anyagok szerkezetvizsgálata MQMAS NMR módszerrel, KUE 95, Akadémiai Kiadó, Budapest, 2006.
Kovács I., Szőke J.:Molekulaspektroszkópia, Akadémiai Kiadó, Budapest, 1987.
S. Berger, S. Braun: 200 and More NMR Experiments, Wiley-WCH, 2004.

Title of the course: Molecular spectroscopy laboratory

Credits: 6

Coordinator/Department: György Tarczay / Department of Inorganic Chemistry

Terms for joining: Fulfilement of courses "Modern Structural Research Methods" and "Laboratory Praxis of Modern Structural Research Methods"

Topics covered by the course:
The aim of this course is the detailed study of the experimental aspects of the optical spectroscopic methods, as IR-, Raman-, UV/VIS-, UPS- and CD-spectroscopy.
This course focuses on the methodology, the data acquisition steps and the software applied as well as the interpretation of the results. Some typical examples are used to demonstrate the ability of the mentioned experimental methods. At the end of this course the student will be able to plan, perform experiments as well as to treat and evaluate the acquired data on his/her own.

Literature*:
Compulsory:

Suggested:
Kovács I., Szőke J.:Molekulaspektroszkópia, Akadémiai Kiadó, Budapest, 1987.
Holly Sándor, Sohár Pál: Infravörös spektroszkópia, Műszaki Kiadó, 1968.
B. Schrader (szerk.): Infrared and Raman Spectroscopy, Methods and Applications, VCH, 1995

Name of the course: NMR spectroscopy I. : Theory of NMR spectroscopy

Credit: 2
Name of the lecturer/Dept.: Pál Sohár / Dept. of General and Inorganic Chemistry
Terms of joining: Passed oral examinations in Phys.-Chem. & Org. Chem.

Content of the course:
1. Basic theory. Magnetic properties of particles - Magnetic and angular momentum and their quantized nature - The Larmor precession - Magnetic levels and transitions - Population of energy levels - Boltzman distributions - Spin temperature - Relaxations - Saturation - Natural line width - Bloch equations - Signal intensity.

2. The chemical shift. Definition - Its theoretical calculation, contributing factors: dia- and paramagnetic contributions, anisotropic effect of neighbouring groups - Intramolecular (aromatic) ring currents- Additivity of chemical shifts, correlations tables - Chemical shifts scales, calibration.

3. Spin-spin interactions, coupling constants. First-order splitting, multiplicity and intensity rules- Coupling constants and the factors influencing their magnitudes - Higher-order interactions - H-H couplings via two and three chemical bonds, long-range couplings - Chemical and magnetic equivalences, spin systems.

4 . Quantum chemical interpretation of the NMR spectra - The Schrödinger equations of spin-systems - The Hamilton operator - Spin-angular momentum operators - Eigen-functions of the spin systems- Multi-spin systems - Selection rules - Transition probabilities and the relative intensity of spectral lines.

5. Quantum chemical treatment of the most common spin-systems. A2 - AX - AB - AX2 - AB2 - A2X2 - A2B2 - AX3 - AB3 - A2X3 - A2B3 - AMX - ABX - ABC - AA'XX' - AA'BB' . Theoretical spectra. Determination and calculation of spectral parameters.

Compulsory reading (in Hungarian):

Sohár, P.: NMR Spectroscopy, I. Theory of NMR spectra. (Lecture notes). Tankönyvkiadó, Budapest, 1975

Sohár, P: Exercises, I. To the facultative course „NMR spectroscopy" in the autumn semester (Theory of NMR Spectroscopy). (Lecture notes). Tankönyvkiadó, Budapest, 1981, 2nd edition, 1996.

Sohár, P.: NMR Spectroscopy, I-II. Akadémia Kiadó, Budapest, 1976

Recommended literature:

J. T. Clerc, E. Pretsch, J. Seibl: Structural Analysis of Organic Compounds by Combined Application of Spectroscopic Methods.

Name of the course: NMR spectroscopy II: Applications in structure elucidation

Credit: 2
Name of the lecturer/Dept.: Pál Sohár / Dept. of General and Inorganic Chemistry
Required previous studies: Passed oral examinations in NMR spectroscopy, I.

Content of the course:
1H NMR spectroscopy. Saturated open-chain, cyclic and hetero cyclic compounds - Olefines and acetylenes - Aromatic compounds - Hetero aromatic compounds - Spectra of flexible molecules containing mobile hydrogens - Signal shape-analysis - Determination of thermodynamic parameters by NMR.

2. 13C NMR spectroscopy. The factors influencing the carbon chemical shifts - Field effect - C-NMR properties of different groups of compounds. - Couplings of carbon nuclei - Carbon relaxations - Carbon relaxation mechanisms.

3. Medium effects in the NMR spectroscopy. Solvent effects - Shift reagents - Chemically induced dynamic nuclear polarisation (CIDNP).

4. NMR measuring methods. CW spectrometers - Spectrum integration - Variable temperature measurements - FT-spectroscopy - Pulsed excitation - Computer controlled spectrometers - Double resonance - NOE - Gated decoupling - Pulse sequences - DEPT (determination of the order of carbon atoms) - Measurement of relaxation times.

5. 2D-NMR spectroscopy. COSY (proton-proton correlation via couplings) - HSC (hetero-nuclear shift correlation : signal matching) - NOESY (NOE-correlation) - NMR-imaging: Medical applications.

Compulsory reading (in Hungarian):
Sohár, P.: Selected topics of up-to-date NMR spectroscopy. Recent results in the chemistry, 58. (Ed.: Csákvári, B.). Akadémia Kiadó, Budapest, 1984
Sohár, P.: Carbon Resonance Spectroscopy, 59 (Ed.: Csákvári, B.). Akadémia Kiadó, Budapest, 1984
Sohár, P.: Nuclear magnetic resonance spectroscopy, I-II. Akadémia Kiadó, Budapest, 1976

Recommended literature:
A. E. Derome: Modern NMR Techniques for Chemistry Research. Pergamon Press, Oxford, 1987
E. Breitmaier: Structure Elucidation by NMR in Organic Chemistry. Wiley, 1993
J. K. M. Sanders and B.K. Hunter: Modern NMR Spectroscopy. Oxford Univ. Press, 1987

Title of the course: NMR Spectroscopy of Solids

Credits: 2

Coordinator/Department: Dr. János Rohonczy / Department of Inorganic Chemistry

Terms for joining: Fulfilement of course "NMR Spectroscopy" by J. Rohonczy

Topics covered by the course:

Topics: magnetic interactions in solids, their effects on NMR spectra and their description by irreducible spherical tensors. Homo- and heteronuclear decoupling and recoupling methods. Magnetic interactions at magic angle spinning. The theory and practical hints of the cross-polarization experiments. Experimental aspects of the measurement of half integer spin nuclei by DAS, DOR, MQMAS and STMAS techniques. The theoretical limitation of the measurement of integer spin nuclei. Correlation 2D experiments in solids.

Literature*:

Compulsory:

Suggested:

Rohonczy J.: Szilárd anyagok MQMAS NMR vizsgálata,
A kémia újabb eredményei 95, 2005, Akadémiai Kiadó, 2006.
S. Berger, S. Braun: 200 and More NMR Experiments, Wiley-WCH, 2004.
K.J.D. MacKenzie, M.E.Smith, Multinuclear Solid-State NMR of Inorganic Materials, Pergamon Press, 2002. (ISBN 0-08-043787-7)

Title of the course: Optical spectroscopy

Credits: 2

Coordinator/Department: Gabor Magyarfalvi, Department of Inorganic Chemistry

Terms for joining:

Topics covered by the course: Basic concepts of ultraviolet, visible, infrared, Raman and fluorescence spectroscopy. Basic theory of electronic transitions and molecular vibrations. Principles and operation of spectrometers. Sample preparation, measurement techniques, coupled methods. Evaluation and assignment of spectral features.

Literature*:
Compulsory:

Suggested:

- Holly Sándor, Sohár Pál: Infravörös spektroszkópia, Műszaki , 1968
- Kovács István, Szőke József: Molekulaspektroszkópia, Akadémiai , 1987
- Sztraka Lajos: A Fourier-transzformációs spektrometria elvi alapjai, A kémia újabb eredményei 36, Akadémiai, 1977
- Ruff Ferenc: Szerves vegyületek szerkezetvizsgálata spektroszkópiai módszerekkel: Infravörös Spektroszkópia; Szerves vegyületek szerkezetvizsgálata spektroszkópiai módszerekkel: UV-látható spektroszkópia, Tankönyvkiadó, 1992
- J. M. Hollas: Modern Spectroscopy, Wiley, 1998
- D. C. Harris, M. D. Bertolucci: Symmetry and Spectroscopy, An Introduction to Vibrational and Electronic Spectroscopy, Oxford University P., 1978
- E. B. Wilson, J. C. Decius, P. C. Cross: Molecular Vibrations, The Theory of Infrared and Raman Vibrational Spectra, General Publ. Comp., 1955 (Dover)
- B. Schrader (szerk.): Infrared and Raman Spectroscopy, Methods and Applications, VCH, 1995

Title of the course: Pattern Formation in Chemical and Biological Systems

Credits: 2

Coordinator: Szalai, István

Department: Department of Analytical Chemistry

Prerequisites: basic knowledge in mathematics and physics (for those having an ELTE Chemistry BSc: Basics of Mathematics for Chemists (KAMAT1, KAMAT2), Physics I. (KAFIZ1); for others: equivalent knowledge)

Topics covered by the course:
Pattern formation in nonlinear chemical and biological systems. Nonlinear thermodynamics. Instabilities in nonlinear systems. Stability analysis. Kinetic and diffusion driven instabilities in reaction-diffusion systems. The activator-inhibitor model. Deterministic chaos in chemistry and biology.

Literature:
Compulsory:
Pontrjagin: Közönséges differenciálegyenletek (Akadémiai Kiadó, 1972)
Tél-Gruiz: Kaotikus Dinamika (Nemzeti Tankönyvkiadó, 2002)
Nemlineáris dinamika és egzotikus kinetikai jelenségek kémiai rendszerekben (egyetemi jegyzet, Szerkesztő: Dr. Bazsa György, Debrecen-Budapest-Gödöllő, 1992)
Suggested:
Murray: Mathematical Biology (Springer, 2002)
Camazine, Deneubourg, Franks, Sneyd, Theraulaz, Bonabeau: Self-Organization on Biological Systems (Princeton Universyti Press, 2003)

Title of the course: Practice in molecular sensors

Credit: 4

Coordinator /Department: Péter Kele research associate, Department of Inorganic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in analytical, inorganic and organic chemistry (successful exams in analytical, inorganic and organic chemistry, for others: equivalent knowledge). Successful exam in Principles of molecular recognition is a prerequisite.

Topics covered by the course:
Design and synthesis of fluorescent sensors for targeted analytes. Completion of multi step syntheses (literature search, synthesis planning, isolation of intermediates, purification of intermediates, isolation of product, purification of product, structure verification)
Spectrophotometric and fluorimetric testing of the switches produced.

Suggested literature:
Chem. Rev. **1997**, *97*, 1515; Valeur, B. *Molecular Fluorescence*, Wiley-VCH, Weinheim, 2001; *Chem. Eur. J.* **2004**, *10*, 574;

Title of the course: Principles of Molecular recognition

Credits: 2

Coordinator/Department: Peter Kele / Department of Inorganic Chemistry

Terms for joining:

Topics covered by the course:
The basics of molecular recognition is introduced to the students on examples that are mainly based on fluorescence sensors. In the course of the lectures the following topics are discussed: principles of fluorescence, n-πsensors, internal charge transfer (ICT) sensors, photoinduced electron transfer (PET) sensors, dual sensing (TICT), excimer based sensors, Energy transfer systems, chiral recognition, logic gates, sensor applications of quantum dots (QD). Besides the working principles of the sensors mentioned above, receptors of specific analytes are also discussed (alkali, alkali earth, transition metals, small organics, sugars, amino acids, nucleic acids).

Literature*:
Compulsory:

Suggested:

Title of the course: Reactions of metal complexes in Solution: Kinetics and Mechanism

Credits: 2

Coordinator: Simándi, László

Department: Department of Analytical Chemistry

Prerequisites: admission to Chemistry MSc, basic knowledge in inorganic and physical chemistry

Topics covered by the course:
Basics of coordination chemistry. Reactions of metal complexes in solution: complex-forming and ligand exchange reactions. Mechanism of ligand substitution: dissociation, association and exchange. Redox reactions. Outer- and inner-sphere electron exchange, atom exchange. Kinetics and thermodynamics.

Literature*:
Compulsory:
Simándi László: Fémkomplexek oldatreakció. Kinetika és mechanizmus (handout)
Suggested books:
selected articles

Title of the course: Sol-gel method

Credits: 2

Coordinator: Sinkó, Katalin

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in inorganic and colloid chemistry

Topics covered by the course:

The sol-gel method is able to produce glass and ceramic materials by a low energy-consuming technique replacing the high energy-consuming traditional melting processes. On the other hand, the sol-gel method is a very good tailoring technique for preparation of materials with controlled structures and properties. The course covers the chemical processes (hydrolysis, condensation) of the silicate systems, the gelation processes of the non-silicate based systems (aluminate, borate, zirkonate, titanate systems) the kinetic of gelation, the drying and sintering processes of gels, the comparison of the products produced by traditional melting and sol-gel techniques, and the application possibilities.

Literature:

Brinker, C. J.; Scherer, G. W. *Sol-gel Science*; Academic Press: Boston, 1990.
J. W. Martin: The Structure of Materials, Elsevier, Amsterdam 2007.

Suggested books:
R. W. Cahn: The coming of materials science, Pergamon, Amsterdam,
W. D. Callister: Materials Science and Engineering, An Introduction, Wiley,
W.F. Smith: Principles of Materials Science and Engineering, McGraw-Hill Publ.

Title of the course: Structure and Properties of Metals and Alloys

Credits: 2

Coordinator: Kuzmann, Ernő

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in physics and thermodynamics

Topics covered by the course:

Selected topics in metal physics and physical metallurgy. Electron structure of metals. Crystal structures. Atomic radii. Crystal lattices of metals. Defects. Alloys. Primary solid solutions. Intermetallic compounds. Phase diagrams. Phase transitions. Amorphous alloys. Electrical properties of metals and alloys. Superconductivity. Magnetic properties of metals and alloys.

Literature:
Suggested books:
C.S. Barrett, T.B. Massalski, Structure of Metals, *MacGraw Hill*, London ,1966
J. Verő, M. Káldor, Fémtan, Nemzeti Kiadó, Bp, 1977.
Ch. Kittel, Bevezetés a szilárdtestfizikába, Müszaki Kiadó, Bp, 1981.
A.G.Guy, Fémfizika. Műszaki Kiadó. Bp. 1978.

Title of the course: Systematic Organometallic Chemistry

Credits: 2 credits

Coordinator/Department: László Szepes Professor in Chemistry

Department of Inorganic Chemistry

Terms for joining: general entrance requirements of Chemistry MSc program, basic knowledge

in Organometallic Chemistry (In the case of completed ELTE BSc courseprerequisite is

Organometallic Chemistry (kv1n1en5), or equivalent in any other case.)

Topics covered by the course:
the course place an equal emphasis on main group element and transition metal organometallic chemistry including preparative methods, structural and bonding problems, spectroscopy, as well as selected highlights of the most recent research and applications.

Literature:
Faigl, F., Kollár, L., Kotschy, A., Szepes, L., Szerves Fémvegyületek Kémiájа, Nemzeti Tankönyvkiadó, Budapest, 2001. (Hung.)
Elschembroich, Ch., Salzer, A., Organometallics, VCH, Weinheim, 2nd (or more recent) edition, 1992.
Cotton, F.A., and Wilkinson, G., Advanced Inorganic Chemistry, John Wiley, New York, 5th (or more recent) edition, 1988.

Title of the course: Spectroscopic Application of Photoionization

Credits: 2 credits

Coordinator/Department: László Szepes Professor in Chemistry

Department of Inorganic Chemistry

Terms for joining: general entrance requirements of Chemistry MSc program, basic knowledge

in Theoretical Chemistry and Spectroscopy (In the case of completed ELTE BSc course

prerequisite is Theoretical Chemistry (kv1n1lm1), or equivalent in any other case.)

Topics covered by the course:
the course covers the main principles of photoionization; the basic concepts and applications of UV photoelectron spectroscopy (UPS, XPS) and related techniques, like photoelectron-photoion coincidence experiment (PEPICO), zero kinetic energy spectroscopy (ZEKE), and special features of photoionization mass spectrometry (PIMS).

Literature:
Borossay J., Szepes L., Fotoelektron-spektroszkópia. Molekulaspektroszkópia, Szerk.: Kovács I., Szőke J., Akadémiai Kiadó, Budapest, 1987, 719-761. (Hung.)
Eland, J.H.D., Photoelectron Spectroscopy, Butterworth, London, 1974.
Briggs, D. (Ed.), Handbook of X-ray and Ultraviolet Photoelectron Spectroscopy, Heyden, London, 1977.
Müller-Detlefs, K., High Resolution with Photoelectrons: ZEKE Spectroscopy of Molecular Systems, in *High Resolution Laser Photoionization and Photoelectron Studies*, (Powis, I., Baer, T., Ng, C-Y., Editors), Wiley, 1995, pp. 21-70.
Baer, T., Booze, J., and Weitzel, K.-M., Photoelectron-Photoion Coincidence Studies of Ion Dissociation Dynamics, in *Vacuum Ultraviolet Photoionization and Photodissociation of Molecules and Clusters*, (Ng, C-Y., Ed.) World Scientific, Singapore, 1991, pp. 259-296.

Title of the course: Vacuum Technology

Credits: 2

Coordinator/Department: Assistant prof. David Frigyes,

Dept. of Inorganic Chemistry

Terms for joining: -

Topics covered by the course:
History of vacuum technology, theoretical basis (kinetic gas theory, impact numbers, heat transfer and electrical conductivity of gases), vacuum-compatible and vacuum-incompatible materials, vacuum pumps and gauges, standards, vacuum troubleshooting

Literature*:
Compulsory:
http://vacutech.elte.hu

Suggested:
Saul Dushman (Editor), James M. Lafferty, Scientific Foundations of Vacuum Technique, John Wiley & Sons Inc; 2Rev Ed edition (December 1962)

Organic Chemistry - specialized module

Title of the course: Advanced synthetic organic chemistry

Credit: 2
Coordinator /Department: István Jalsovszky, associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exams in organic chemistry and laboratory practices, for others: equivalent knowledge)

Topics covered by the course: Effective methods to build carbon-carbon bonds; Functional group transformations; Retrosynthetic analysis; Surprising experimental facts by using well-known reactions in laboratory practice.

Suggested literature:

Richard C. Larock: Comprehensive Organic Transformations (VCH, ISBN: 3-527-26953-3)

Title of the course: Adverse health effect of chemicals and their prevention

Credits: 2

Coordinator: Marcsek, Zoltán

Department: Department of Molecular and Cell Biology, National Institute of Chemical Safety

Prerequisites: admission to Chemistry and/or Biology MSc, basic knowledge in chemistry and/or biology

Topics covered by the course:
Risk of using chemicals, sustainable growth and wide use of chemicals, the ’chemical safety’. Getting chemicals into the living organisms, their effect on the organs. Structure-activity relationship. Toxicological tests: principles, levels: animal and non-animal (in vitro) systems. Acute toxicity, ’late toxic effects’: tumor promotion, genotoxic, immunotoxic effects, endocrine disrupters, neurotoxins, effect on reproductive organs and pre/neonatal development. Substances acting against living organisms: biocides, herbicides, production enhancers. Categorization of toxic chemicals, intoxications. National (OKBI) and international institutions (EU: REACH, OECD, USA/Japan: EPA), risk of production, treatment and distribution of chemicals, risk assessment.

Literature*:
Compulsory:
Tompa Anna (ed): Kémiai biztonság és toxikológia. Medicina Kiadó, Budapest, 2004.

Suggested:
Kopper László, Marcsek Zoltán, Kovalszky Ilona: Molekuláris medicina. Medicina Kiadó, Budapest, 1997.

Title of the course: Analogue-based drug research

Credit: 2

Coordinator /Department: Zsuzsa Majer – Department of Organic Chemistry

Terms for joining: BSc in chemistry, for others: equivalent knowledge of organic chemistry and biochemistry

Topics covered by the course:
Analogues as Means of Discovering New Drugs. Privileged Structures and Analogue-based Drug Discovery. Case History of Omeprazole-Esomeprazole and Pantoprazole. Optimizing antihypertensive Therapy by Angiotensin Receptor Blockers. Case Study of Lacidinpine in the Research of New Calcium antagonists. Selective Beta-Adrenergic Receptor blocking Agents. Development of Organic Nitrates for Coronary Heart Disease. Development of Opioid Receptor Ligands. Cisplatin and Its Analogues for Cancer Chemotherapy. Corticosteroids; from Natural Products to Useful Analogues

Literature*:
Analogue-based Drug Discovery (Editors: J. Fischer and C.R. Ganellin
Wiley-VCH (2006)
ISBN 3-527-31257-9

Title of the course: Application of thermal decomposition reactions for waste recycling

Credits: 2

Coordinator/Department: Marianne Blazsó/ Department of Organic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in polymer chemistry

Topics covered by the course:
Thermally initiated chemical reactions in organic materials. Thermal decomposition of organic macromolecules. Organic macromolecular materials in industrial, agricultural and communal waste. Thermal decomposition reactions of synthetic polymers (poliolefins, vinyl polymers, PVC, rubbers, polyethers, polyesters, polyamides, polyurethanes, phenolic resins, epoxy resins, siliconorganic polymers). Thermal decomposition of wood, biomass, cellulose and lignin. Catalytic upgrading of the pyrolysis oils of plastics and biomass. Pyrolysis of wastes in coal and petroleum industry, catalytic upgrading of the pyrolysis oils.

Literature*:
Compulsory:

Suggested:
Feedstock recycling and pyrolysis of waste plastics, (Scheirs, Kaminsky Eds., Wiley, 2006)

Name of the course: Asymmetric Synthesis

Credit: 2

Coordinator /Department: Géza Timári, Chinoin Co. Ltd.

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Practical method of stereoselective synthesis with emphasis on recent advantages. It embraces a wide variety of subjects, such as hydrogenation over chiral catalysts, stereoselective epoxidation and dihydroxylation. Assymetric carbon-carbon bond formation.

Compulsory literature:
Mihály Nógrádi, Stereoselective Synthesis, VCH, 1995

Suggested literature:
A. Kotschy, G. Timári, Heterocycles from Transition Metal Catalysis, *Springer*, 2005

Title of the course: Biomolecular chemistry II

Credit: 2

Coordinator /Department: Miklós Hollósi professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and biochemistry (successful exams in organic and biomolecular chemistry, for others: equivalent knowledge)

Topics covered by the course:
Exploring proteins. Exploring genes. Recombinant DNA technology. Lipids and cell membranes. Membrane channels and pumps. Metabolism: basic concepts and design. Signal-transduction. Metabolism of fatty acids. Protein turnover and amino acid catabolism. Synthesizing the molecules of life. Responding to environmental changes

Compulsory literature*:
M. Hollósi., B. Asbóth, Biomolekuláris kémia II, Nemzeti Tankönyvkiadó, Budapest, 2007

Suggested literature:
J.M. Berg., J.L. Tymoczko, L. Stryer, Biochemistry, fifth edition, W.H. Freeman and Co., New York, 2002

Title of the course: Biomolecular Mass Spectrometry

Credit: 2

Coordinator /Department:

Gitta Schlosser, Research Group of Peptide Chemistry, Department of Organic Chemistry

Terms for joining: R

Requirements of the Chemistry M.Sc., basic knowledge in analytical and organic chemistry (successful exams in analytical and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:

1. Basic concepts of mass spectrometry (ionization methods, analyzers)
2. Tandem mass spectrometry (MS/MS), peptide sequencing
3. Coupling of separation techniques with mass spectrometry
4. Structural characterization of peptides, proteins, oligonucleotides, oligosaccharides and lipids
5. Protein identification, protein quantification, identification of post-translational modifications, proteomics
6. New perspectives in mass spectrometry

Compulsory literature*:

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Suggested literature:

1. Chhabil Dass: **Principles and Practice of Biological Mass Spectrometry** (Wiley)

2. Chava Lifshitz , Julia Laskin: **Principles of Mass Spectrometry Applied to Biomolecules** (Wiley)

3. Mahmoud H. Hamdan, Pier G. Righetti: **Proteomics Today: Protein Assessment and Biomarkers Using Mass Spectrometry, 2D Electrophoresis, and Microarray Technology** (Wiley)

Title of the course: **BioNMR spectroscopy**

Credits: **3 lectures and 2 practicals / week, 5 credit**
Credit number: **5**
compulsory lecture for every students having BSc

Coordinator: **Perczel András**

Department: **Organic Chemistry**

Closing the course: **colloquium**

Topics covered by the course:

The aim of the lecture is to introduce the theory and practice of NMR-spectroscopy of organic and biomolecules. The principles of how to evaluate complex spectra and structure elucidiation are provided.
Theoretical basis of bio-NMR spectroscopy are given such as: the vector model, the product operator formalism, relaxation, nuclear Overhauser effect, polarisation transfer, scalar and dipolar coupling, population and coherence transfer, chemical shift *etc.*.
NMR signal assignment and multidimensional NMR spectroscopy (e.g. COSY, RELAY, TOCSY, NOESY, ROESY) is introduced.
Isotope labelling and spectral editing strategies (e.g. HSQC, HMBC, TOCSY-HSQC, HNCO, HNCA) are outlined.
Basics of NMR structure calculation will be described, including data collection, resonance assignment, collection of structural restraints, targetfunction minimalisation and quality assessment.
Different approches related to structure determination of proteins (smaller than 15 kDa, 15-30 KDa and larger than 30 kDa) are described.
Comparison of NMR- and X-ray determined structures are given.
Protein folding is introduced viewed by NMR specroscopy: namely thermal unfolding, hydrogen-deuterium exchange, intrinsically unstructured proteins etc..
Enzymes and their function, as seen by NMR spectroscoy.
NMR spectroscopy of nucleic acids and carbohydrates will also be introduced briefly.

Compulsory literature: P.J. Hore NMR spectroscopy (Nemzeti Tankönyvkiadó, 2003)
E-Notes of the lecture
Suggested literature: J.N.S.Evens *Biomolecular NMR Spectrscopy* (Oxford Univ. Press. 1995)
A.K.Downing *Protein NMR techniques* Second Ed. (Humana Press 2004)

Title of the course: Bioorganic chemistry

Credit: 2

Coordinator /Department: Kalman Medzihradszky, Organic Chemistry

Terms for joining: *requirements of the Chemistry Msc., basic knowledge in inorganic and organic chemistry (successful exams in inorganic and organic chemistry, for others: equivalent knowledge)*

Topics covered by the course:
Pharmacokinetics: Drug distribution, binding to macromolecules, separation techniques, affinitiy chromatography
Metabolism: Drug labeling with radioisotopes, microsomal conversion, conjugation reactions, prodrug-drug conversion, biosynthesis of peptide hormones
Chemotherapy: Structure of the bacterial cell wall, antibacterial compounds, antibiotics, cancer chemotherapy
Pharmacodynamics: Structure and function of receptors, inhibition of proteolytic enzymes, opioid peptides

Compulsory literature: —

Suggested literature:W.O.Foye (Ed): Principles of Medicinal Chemistry, Lea and Fabiger, Philadelphia-London, 1989.

Name of the course: Biospectroscopy laboratory

Credit: 4

Coordinator/Department: Elemér Vass, associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and spectroscopy [successful exams in organic chemistry (2) and organic spectroscopy, for others: equivalent knowledge]

Topics covered by the course:

The aim of the course is to acquire practical skills in the most important spectroscopic methods used in the structure analysis of biomolecules (such as peptides, proteins, steroids and nucleic acids). The course also provides the basic knowledge necessary for the interpretation of spectra and the determination of the steric structure. The subject consists of ultraviolet-visible (UV-VIS), infrared (IR), bioNMR, biomolecular mass spectrometry, as well as electronic and vibrational circular dichroism (CD, VCD) laboratory courses.

Compulsory literature:
Műszeres Szerves Analitikai Gyakorlatok, Egyetemi jegyzet, összeállította az ELTE Szerves Kémiai Tanszék munkaközössége, Budapest (1995).
Joseph B. Lambert, Herbert F. Shurvell, David A. Lightner, R. Graham Cooks: Organic Structural Spectroscopy, Prentice Hall, Upper Saddle River, New Jersey, USA (2001)

Suggested literature:
Hollósi Miklós, Laczkó Ilona, Majer Zsuzsa: A sztereokémia és kiroptikai spektroszkópia alapjai, Nemzeti Tankönyvkiadó, Budapest (2004).
Perczel András, Laczkó Ilona, Hollósi Miklós: Peptidek térszerkezet-vizsgálata. A kémia legújabb eredményei, Akadémiai Kiadó, Budapest (1994).
Gerald D. Fasman (Ed.): Circular Dichroism and Conformational Analysis of Biomolecules, Plenum Press, New York (1996).

Name of the course: Chemical and functional characterisation of biologically active peptides *in vitro*

Credit: 1

Coordinator /Department: Szilvia Bősze, Research Associate Professor, HAS-ELTE Research Group of Peptide Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exams in organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Chemical characterisation of peptides and peptide derivatives (amino acid analysis, sequencing, determination of the substitution degree). Elemental analysis, determination of fluorescence parameters. Cellular uptake studies (concentration, time- and temperature dependency). Cytotoxicity studies.

Compulsory literature*:
Cooper, C: Amino Acid Analysis Protocols, (chapters) Humana Press, 2000
Walker, JM: Basic Protein and Peptide Protocols, (chapters) Humana Press, 1994
Walker, JM: Protein Protocols, (chapters) Humana Press, 2002
Suggested literature:
Az elemanalitika korszerű módszerei Akadémiai Kiadó, 2006, (szerk. Záray Gyula).
Immunológiai módszerek, Medicina 2007, szerk: Erdei Anna

Name of the course: Chemical and functional characterisation of biologically active peptides *in vitro,* laboratory practice

Credit: 1

Coordinator /Department: Szilvia Bősze, Research Associate Professor, HAS-ELTE Research Group of Peptide Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exams in organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Amino acid analysis of synthetic peptides using pre-column and post-column derivatisation techniques (SYKAM instrument, RP-HPLC). Elemental analysis using VARIO EL instrument. Cellular uptake studies with using BD LSR II instrument and FACS Diva 5.0 software. Cytotoxicity studies using MTT assay and flow cytometry methods.

Compulsory literature*:
Cooper, C: Amino Acid Analysis Protocols, (chapters) Humana Press, 2000
Walker, JM: Basic Protein and Peptide Protocols, (chapters) Humana Press, 1994
Walker, JM: Protein Protocols, (chapters) Humana Press, 2002
Suggested literature:
Az elemanalitika korszerű módszerei Akadémiai Kiadó, 2006, (szerk. Záray Gyula).
Immunológiai módszerek, Medicina 2007, szerk: Erdei Anna

Title of the course: Chemical informatics in drug design

Credit: 2

Coordinator /Department: Ödön Farkas, associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in general, organic and biochemistry, basic informatics skills.

Topics covered by the course:
The concept of molecules. Representation and modeling of molecular structures and their properties. Conventional naming and coding of chemical structures. Chemical data bases and their management. Fast approximation of molecular properties. QSAR and its application for drug design. Design and validation of models. The concept of pharmacophores. High throughput screening methods. Combinatorial virtual chemistry. Computer aided drug design.

Compulsory literature: -
Chemical informatics in drug design (lecture notes, Department of Organic Chemistry, Eötvös Loránd University, in preparation)
Suggested literature:
Arup K. Ghose, Vellarkad N. Viswanadhan: Combinatorial Library Design and Evaluation: Principles, Software Tools, and Applications in Drug Discovery (ISBN 0824704878), 2001
Gasteiger, Johann / Engel, Thomas (Szerk.): Chemoinformatics. Wiley-VCH, Weinheim, 2003
Examples, presentations and computer programs: http://www.chemaxon.com

Title of the course: Chemical Process Engineering

Credit: 2

Coordinator /Department: István T. Horváth Professor of Chemistry, Department of Organic Chemistry

Terms for joining: basic knowledge in mathematics, physical, inorganic and organic chemistry (successful exams in mathematics, physical, inorganic and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Program: Introduction to the chemical process engineering. Chemical reactors. Separation processes: distillation, adsorption, absorption, extraction, membrane separation. Drying. Hydrodynamic processes: filtration, micro filtration, settling, dust separation, droplet separation. Combined separation processes. Preparative chromatography. Heat exchange. Introduction to the process controlling.

Compulsory literature*:
Gerecs Árpád: Bevezetés a kémiai technológiába, Nemzeti Tankönyvkiadó, Budapest, 1973;
Fonyó – Fábri: Vegyipari Művelettani Alapismeretek, Nemzeti Tankönyvkiadó, Budapest, 1998.
Suggested literature:
Perry: Chemical Engineers' Handbook, Műszaki Könyvkiadó, Budapest 1968.

Title of the course: Chemistry of Organic Fluorine Compounds

Credit: 2

Coordinator /Department: József Rábai, Associate Professor of Chemistry, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc, basic knowledge in inorganic and organic chemistry (successful exams in inorganic and organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
History of fluorine compounds. Properties of fluorine and fluorine compounds. Nomenclature and spectroscopy. Effect of fluorine and fluorine containing substituents on reaction rates. Basic methods for the preparation of organofluorine compounds. Selective and exhaustive fluorinations. The role of fluorine in agrochemicals and pharmaceuticals. Fluorine chemistry and 'performance chemicals'. Introduction of ^{18}F into PET diagnostics. Basics of fluorous biphasic catalysis and fluorous chemistry. Fluorophilicity, lipophilicity and molecular structure. Use of inorganic and organic fluorine compounds for organic syntheses.

Compulsory literature*:

(1) Horváth, I. T.; Rábai, J. *Science* **1994,** *266,* 72 ; idem: US Patent 5,463,082, **1995**; *Chem. Abstr*. **1995,** ***123***, 87349; (3) Horváth, I. T.; et al. *J. Am. Chem. Soc.* **1998,** *120,* 3133; (4) Curran, D. P., et al. *Science* **1997,** *275,* 823; (5) Curran D. P., et al. *Science* **2001,** *291,* 1766.

Suggested literature:

(1) Handbook of Fluorous Chemistry, Eds.: J. A. Gladysz, D. P. Curran, I. T. Horváth; Wiley-VCH, Weinheim, 2004.

(2) FLUORINE, the First Hundred Years (1886-1986), Eds.: R. E. Banks, D. W. A. Sharp, J. C. Tatlow; Elsevier Sequoia, Lausannae and New York, 1986.

(3) Chemistry of Organic Fluorine Compounds, 2nd ed., M. Hudlicky; Ellis Horwood and Prentice Hall, New York, 1976, 1992.

(4) Organofluorine Chemistry — Principles and Commercial Applications, Eds.: R. E. Banks, B. E. Smart, J. C. Tatlow; Plenum, New York, 1994

(5) Fluorine Compounds — Chemistry and Applications; N. Ishikawa, Y. Kobayashi; Kodansha Scientific, 1979

Title of the course: Combinatorial chemistry

Credit: 2

Coordinator /Department: Gábor Dibó associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry M.Sc., basic knowledge organic chemistry (successful exams in organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Combinatorial synthesis strategies (parallel & split–mix). One-bead one-peptide approach. Deconvolution methods. High-throughput synthesis in multimilligram quantities. Synthesis on membrane support. Resins and anchors for solid phase organic synthesis. Diversity- and target-oriented organic syntheses. Analytical methods in combinatorial chemistry. Multi-component reactions. Multi-step solution phase combinatorial synthesis. Experimental techniques in combinatorial fluorous synthesis. Automated solution phase synthesizers. Discovery of new catalysts by combinatorial synthesis. High-throughput screening assays. Combinatorial chemistry in drug discovery. Basic principles of chemical biology.

Compulsory literature:
Fenniri H.: Combinatorial Chemistry — A Practical Approach, *Oxford University Press,* 2000

Suggested literature:
Furka Á: History of Combinatorial Chemistry, *Drug Development Research,* **1995,** *36,* 1–12.
Furka Á, Bennett WD: Combinatorial libraries by portioning and mixing, *Comb. Chem. High Throughput Screening,* **1999,** *2,* 105–122.

Title of the course: Computational neuroscience

Credits: 2

Coordinator/Department: Krisztina Szalisznyo, MD, PhD

Terms for joining: Basic knowledge in analysis, linear algebra and in differential equaitons is advised but not obligatory

Topics covered by the course:
General introduction to the anatomy, evolution and cellular basis of nervous system

Hodgkin-Huxley formalism, cnductance based models and its simplifications, abstract models

Multicompartmental models, detailed and fenomenological models of synapses, synaptic plasticity

Linear stability analysis, phase-space analysis, FitzHugh-Nagumo-Rinzel model, Morris-Lecar model, Type I and Type II membrane excitability, bursting and spiking models,

XPPaut tutorial,

Information theoretical measures, used in computational neuroscience,

Modeling neurological and psychiatric disorders.(Epilepsy, Parkinson's disease. Schizophrenia)

Biologically inspired learning rules,

Computation with oscillations

Literature (*Compulsory*): *Notes on internet,*
Literature (*Advised*):

Spikes: exploring the neural code:
F. Rieke, D Warland, R. de Ruyter van Steveninck, W. Bialek, (1999)

Theoretical neuroscience:
Peter Dayan, L.F. Abbott, (2000)

Spiking Neuron Models,
Wulfram Gerstner and Werner M. Kistler (2002)

Mathematical Physiology,
James Keener and James Sneyd (1998)

Title of the course: Cyclodextrin chemistry

Credit: 2

Coordinator /Department: Judit Orgoványi, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic and analytical chemistry

Topics covered by the course:

Production and properties of cyclodextrins. Cyclodextrin derivatives. Production and structure of inclusion complexes.
Past, present and future of cyclodextrins.
Industrial application of cyclodextrins: pharmaceutical and food industry.
Cyclodextrins in environment protection. Environment-friendly plant protection. Applications in green chemistry.
Synthesis of cyclodextrin derivatives.
Cyclodextrin polimers and their applications.
Cyclodextrins in analytical chemistry. Thermoanalytical investigation of cyclodextrins and their complexes.
Application of cyclodextrins in capillar electrophoresis as chiral selectors.

Compulsory literature*:

Suggested literature:
J. Szejtli: Cyclodextrins and their inclusion complexes, Akadémiai Kiadó, 1982

Title of the course: Designed synthesis of polymers

Credit: 2

Coordinator /Department: Béla Iván, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and chemical technology (successful exams in organic chemistry and chemical technology, for others: equivalent knowledge)

Topics covered by the course: Fundamentals of polymer chemistry, fundamentals of ideal and quasiliving polymerizations, their application in the synthesis of polymers with different macromolecular topologies, synthesis, analyses, structure, properties and applications of linear, grafted, star-shaped, hyperbranched and dendritic polymers and polymer networks.

Compulsory literature*: Handouts provided during the course

Suggested literature: J. P. Kennedy, B. Iván: Designed Polymers by Carboacationic Macromolecular Engineering: Theory and Practice, Hanser Publishers, Munich, New York, 1992

Name of the course: Drug research

Credit: 2

Coordinator /Department: Dr Ferenc Hudecz / Department of Organic Chemistry

Terms for joining: BSc in chemistry (others: equivalent knowledge in organic chemistry)

Topics covered by the course:
Synthetic strategies in drug research (libraries, semi syntheses, enzymatic syntheses). Structure – function relationship studies, design of experiments, interpretation. Molecule design by chemical informatics, molecular modeling, data bases. Stability studies. Random and high-throughput screening techniques. Studying mechanism of action (receptor binding, enzyme inhibition). Toxicity, biodistribution and metabolism studies. Drug-targeting and drug-delivery systems. Drug formulation. Phases of the clinical trial. Drug registration. Patents. Origin and description of the pharmaceutical industry. History and present state of the Hungarian drug market. Successful Hungarian research.

Compulsory literature*:
R. Ng: Drugs-From Discovery to Approval, Wiley, 2004
R. B. Silverman: The Organic Chemistry of Drug Design and Drug Action, Academic Press, 1992

Suggested literature:
P. Krogsgaard-Larsen, T. Liljefors and U. Madsen: Textbook of Drug Design and Discovery 3rd Edition, Taylor and Frances, 2002
Chi-Jen Lee *et al*.: Development and Evaluation of Drugs: From Laboratory through Licensure to Market, 2nd Edition, 2003
G. Thomas: Medicinal Chemistry: An Introduction, Wiley, 2001
J. Cannon: Pharmacology for Chemists (ACS Professional Reference Book), Oxford University Press, 1999

* Együtt 3-5 könyv, jegyzet.

Title of the course: Fundamentals of macromolecular chemical processes

Credit: 3

Coordinator /Department: Béla Iván, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and chemical technology (successful exams in organic chemistry and chemical technology, for others: equivalent knowledge)

Topics covered by the course: Fundamentals of polymer science, chain polymerizations and step-growth polymerizations, polyadditions (radical, anionic, cationic, group transfer, coordination, metathesis, ring-opening polymerizations), step-growth polymerizations (polycondensation and noncondensative polyreactions), polymer modifications, applications, effects of polymers on the environment.

Compulsory literature: Farkas Ferenc: Műanyagok és a környezet (Polymers and Environment), Akadémiai Kiadó, Budapest, 2000

Suggested literature: G. Odian: Principles of Polymerization, Wiley, New York, 2004

Title of the course: Laboratory safety

Credit: 0 in MSc 2 in BSc

Coordinator /Department: István Jalsovszky, Department of Organic Chemistry

Terms for joining: General admission criteria for chemistry MSc.

Topics covered by the course: Introduction to laboratory safety, incident safety, harms of chemicals, dangerous materials sanitary regulations and protection, application of first aid, protection of laboratory, environment, industrial, hygiene, fire- and explosion defense, fire alarm regulations, precautionary measures against electric, pressure-tight and mechanical equipments, work psychology, ergonomics.

Compulsory literature*: kvvm.hu/ jogszabályok, az ELTE TTK Munkavédelmi szabályzata, Tűzvédelmi szabályzata
(vonatkozó internet honlapok)
Suggested literature: Kiss Dénes: Munkavédelem (BME Vegyészmérnöki Kar, Tankönyvkiadó Budapest)
Bükkösi-Frendl-Perjési: Vegyipari Biztonságtechnikai Kézikönyv (MKE)
OMKTI kiadványok, Országos Munkavédelmi Képző- és Továbbképző Központ biztonságtechnikai könyvsorozata, Budapest
G. Hommel: Veszélyes anyagok, Műszaki Könyvkiadó, Budapest

Title of the course: Methods of Protein Crystallography

Credit: 2

Coordinator /Department: Veronika Harmat research fellow, Department of Organic Chemistry

Terms for joining: -

Topics covered by the course:
Introduction to X-ray diffraction the methods of structure determination of biological macromolecules. A practical approach.

1. Theoretical background, possible implications and limitations.
2. The electron density function and the structure factor.
   Diffraction of X-rays on a crystal lattice
   The crystallographic phase problem
   Symmetry
3. Crystallization and data collection strategies
4. Solving the phase problem
   The Patterson function
   Molecular replacement
   Isomorphous replacement methods
   Use of anomalous dispersion
5. From electron density maps to 2D structure of the molecule: model building and refinement. The model bias
6. Validation of the refined model
7. New directions and challenges in protein crystallography
   Structural genomics
   Large structures and poor crystals
8. Applications in drug discovery
   Structure based and fragment based drug design
9. Mebmrane proteins
10. A molecular movie: time resolved crystallography

Suggested literature:

Blow, David „Outline of Crystallography for Biologists", Oxford University Press 2002
Drenth, Jan „Principles of Protein X-Ray Crystallography" Springer 1999

Title of the course: Modern Mass Spectrometry in Biochemistry

Credits: 2

Coordinator/Department: Pál Szabó

Chemical Research Center, Hungarian Academy of Sciences

Dávid Frigyes

Dept. of Inorganic Chemistry

Terms for joining:

Basic knowledge in organic chemistry

Topics covered by the course:
Introduction: ionization methods and analyzers; sample preparation of micro amounts, examination of intact proteins, enzymatic digestion and chemical cleavage in solution and gel, peptide mapping, sequencing, micro- and nanoscale chromatography, peptide sequencing by means of tandem mass spectrometry, investigation of post-translational modifications (methylation, disulphide bridges, phosphorilation, glycosylation), investigation of protein complexes: determination of active site in enzymes, examination of nucleic acids, examination of metabolites, measurement of metabolic stability, multitarget screening, methods in medical diagnostics

Literature*:
Compulsory:
The slides of the lectures is given for the students:
http://ms.elte.hu/bio
Suggested:

Title of the course: Modern synthetic methods

Credit: 2

Coordinator /Department: András Kotschy associate professor, Department of Inorganic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exams in organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Biocatalysis, syntheses in supercritical media, combinatorial chemsitry, photochemistry, rearrangement reactions, cross-coupling, metathesis, syntheses in alternate solvent systems (ionic liquids, fluorinated solvents)

Compulsory literature*:

Suggested literature:

Title of the course: Modern synthetic methods lab

Credit: 8

Coordinator /Department: András Kotschy associate professor, Department of Inorganic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exam in organic chemistry and passing of organic chemistry lab, for others: equivalent knowledge)

Topics covered by the course:

Computer assisted literature search
Syntheses on micro-scale
Syntheses under inert conditions
Syntheses in non-conventional solvents
Syntheses under extreme conditions
Automated syntheses

Compulsory literature*:

Suggested literature:

Name of the course: MOLECULAR ENGINEERING OF MACROMOLECULES

Credit: 2

Coordinator /Department: Béla Iván h. professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and chemical technology (successful exams in organic chemistry and chemical technology, for others: equivalent knowledge)

Topics covered by the course:

There are two major aims of this course given in English: (1) obtaining fundamental knowledge on modern polymer chemistry and (2) learning the corresponding chemistry, especially polymer chemistry professional terminology in English. The chain polymerization and step-growth polymerization processes and their mechanisms, the ideal living and quasiliving polymerizations and the synthetic applications thereof will be studied.

Compulsory literature*: Handouts provided during the course

Suggested literature: J. P. Kennedy, B. Iván: Designed Polymers by Carboacationic Macromolecular Engineering: Theory and Practice, Hanser Publishers, Munich, New York, 1992.
G. Odian: Principles of Polymerization, Wiley, New York, 2004

Title of the course: Molecular informatics

Credit: 2+2

Coordinator /Department: Ödön Farkas, associate professor, Department of Organic Chemistry

Lecturer(s): Ödön Farkas, Zoltán Gáspári

Terms for joining: requirements of the Chemistry Msc., basic knowledge in general and organic chemistry, basic informatics skills

Topics covered by the course:
The concept and modelling of molecules. Conventional naming and coding of chemical structures. Data bases of chemical structures, properties, experimental data and their management. Fast approximation of molecular properties. QSAR and its application for drug design. The concept of pharmacophores. High throughput screening methods. Combinatorial virtual chemistry. Computer aided reaction design.

Compulsory literature: -
Lecture notes
Suggested literature:
Gasteiger, Johann / Engel, Thomas (Szerk.): Chemoinformatics. Wiley-VCH, Weinheim, 2003
Examples, presentations and computer programs: http://www.chemaxon.com

Title of the course: Name Reactions in Organic Synthesis

Credit: 2

Coordinator /Department: Novak Zoltan, Department of Inorganic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exams in organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Discussion of advanced name reactions in organic synthesis. Reactions, mechanism and applications in the synthesis of complex organic molecules

Compulsory literature*:
Smith, M. B.; March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure

Suggested literature:

Title of the course: **NMR pulses in structure research**

Credits: **2 lectures / week, 2 credit**
Credit number: **2**
suggested lecture for every students having BSc

Coordinator: **Perczel András**

Department: **Organic Chemistry**

Closing the course: **colloquium**

Topics covered by thIS course:

To date, the available high field NMR instruments (12–16 tesla) give the possibility of aquiring spectral information on solution structures of macromolecules (e.g. proteins) as large as 30–50 kDa. With this technical background, NMR spectroscopy heavily contributes to relatively new research fields such as biotechnology, structural biochemistry, molecular biology, virology *etc*.. This course, which does not require any previous knowledge of NMR aims to introduce the basic phenomena of solution state NMR spectroscopy. The goal is to get familiar with the theoretical and practical aspects of one- and multi-dimensional experimenst useful in structure elucidation. First, the vector model is introduced follwed by the description of the product operator formalism. Having these in hand, comlex pulsesequences such as HSQC, HNCA etc. will be explained. During this course additional aspects of modern NMR will be outlined such as relaxation, data prcessing, signal assignment strategies and structure calculation.

Comulsory literature: P.J. Hore "*Magnetic Resonance Spectroscopy*" (Nemzeti Tankönyvkiadó, 2003)
E-notes and handout of the course
Suggested literature: J.N.S.Evens "*iomolecular NMR Spectrscopy"*(Oxford Univ. Press. 1995)
A.K.Downing "P*rotein NMR techniques"* Sec. Ed. (Humana Press 2004)

Title of the course: NMR spectroscopy - applications

Credit: 2

Coordinator/Department: Andrea Bodor, Institute of Chemistry

Terms for joining: basic knowledge in physical chemistry

Topics covered by the course:
The goal of the course is to cover some theoretical aspects of NMR spectroscopy, to clarify and specify the information available from NMR spectra. The student will be capable to decide – especially in the study of small molecules – what type of measurement to run, how to evaluate it in order to answer questions regarding structure and/or dynamic behavior of solution species. Besides theoretical aspects several examples are presented, all of which are possible to perform in the NMR laboratory of Eötvös University.

Compulsory literature:
1. P. J. Hore: Mágneses magrezonancia, Nemzeti Tankönyvkiadó, Budapest, 2004.
2. P.W. Atkins: Fizikai Kémia, Nemzeti Tankönyvkiadó, Budapest, 2001.

Suggested literature:
1. M. H. Levitt: Spin Dynamics, John Wiley & Sons, England, 2001.
2. A. E. Derome: Modern NMR Techniques for Chemistry Research, Pergamon Press, England, 1987.

Title of the course: Organic syntheses from microscale to industrial scale

Credit: 8
Coordinator /Department: István Jalsovszky, associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exams in organic chemistry and laboratory practices, for others: equivalent knowledge)

Topics covered by the course: Solid and liquid phase microscale syntheses; Combinatorial chemistry in 1-2g scale; Organic syntheses using advanced methods in 100 – 500g scale. Scale up in laboratory. Problematic of industrial scale up.

Suggested literature:

Richard C. Larock: Comprehensive Organic Transformations (VCH, ISBN: 3-527-26953-3)

Title of the course: Physical organic chemistry I.

Credit: 2

Coordinator/Department: Elemér Vass, associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry and physical chemistry [successful exams in organic chemistry (2) and physical chemistry (2), for others: equivalent knowledge]

Topics covered by the course:

The course gives an introduction to the fundamental chemical and physical-chemical methods used in the investigation of the mechanism of organic reaction and covers the following topics: Non-kinetic investigation methods of the mechanism of organic reactions. Energetic conditions of organic reactions. Kinetics of elementary reactions. Kinetics of complex reactions. Transition states of chemical reactions. Structure-reactivity relationships.

Compulsory literature:
Ruff Ferenc, Csizmadia G. Imre: Szerves reakciómechanizmusok vizsgálata. Nemzeti Tankönyvkiadó, Budapest (2000).
Suggested literature:
Eric V. Anslyn, Dennis A. Dougherty: Modern Physical Organic Chemistry. University Science Books, USA (2006).
Dr. Szántay Csaba: Elméleti Szerves Kémia, 3. kiadás. Műszaki Könyvkiadó, Budapest (1984).

Name of the course: Physical organic chemistry II.

Credit: 2

Coordinator/Department: Elemér Vass, associate professor, Department of Organic Chemistry

Terms for joining: successful exam in Physical organic chemistry I.

Topics covered by the course:

The course is building on the knowledge-base of Physical organic chemistry I special course and is aimed at teaching advanced physico-chemical theories and reaction kinetic methods used in the investigation of the mechanism of organic reactions. The subject treats the following chapters of physical organic chemistry: Isotope effects. Medium effects. Acids, bases, electrophiles, nucleophiles. Homogeneous catalysis.

Compulsory literature*:
Ruff Ferenc, Csizmadia G. Imre: Szerves reakciómechanizmusok vizsgálata. Nemzeti Tankönyvkiadó, Budapest (2000).
Suggested literature:
Eric V. Anslyn, Dennis A. Dougherty: Modern Physical Organic Chemistry. University Science Books, USA (2006).
Dr. Szántay Csaba: Elméleti Szerves Kémia, 3. kiadás. Műszaki Könyvkiadó, Budapest (1984).

Title of the course: Polymer chemistry lab

Credit: 4

Coordinator /Department: Béla Iván , MTA KKI

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry and chemical technology (successful exams in organic chemistry and chemical technology, for others: equivalent knowledge)

Topics covered by the course: Polymerization experiments, fundamental experimental techniques with polymers, investigation of polymerization kinetics, polymer purification methods, analyses of polymeric materials

Compulsory literature: Handouts provided during the course

Suggested literature:

Title of the course: Principles of stereochemsitry and chiroptical spectroscopy

Credit: 2

Coordinator /Department: Miklós Hollósi professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in organic chemistry (successful exams in organic chemistry and physico-chemsitry, for others: equivalent knowledge)

Topics covered by the course:
Principles of stereochemistry. Stereoisomers. Symmetry. Configuration and conformation. Separation of stereoisomers (resolvation, racemization). Heterotopic ligands and faces. Chiroptical spectroscopy. Applied CD spectroscopy. CD spectroscopic characterization of biopolymers. Vibrational optical activity

Compulsory literature*:
Hollósi, M., Laczkó, I., Majer, Zs. A sztereokémia és kiroptikai spektroszkópia alapjai, Nemzeti Tankönyvkiadó, Budapest, 2004

Suggested literature:
Perczel, A., Laczkó, I, Hollósi, M. Peptidek térszerkezet-vizsgálata A kémia újabb eredményei, Akadémiai Kiadó, Budapest, 1994

Title of the course: Quantum chemistry in practice

Credit: 1+1

Coordinator /Department: Ödön Farkas, associate professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge of theoretical chemistry, basic informatics skills.

Topics covered by the course:
Using quantum chemistry to solve chemical problems, the expected accuracy of the results. Extrapolated and multi-layer models (G2, G3, ONIOM, CBS, etc.), solvent models and periodic boundary conditions. Regular problems during while executing computations, design of computational process. Methods for geometry optimization and computation of trajectories. Topology of potential energy surfaces. Use of Gaussian and GaussView.

Compulsory literature: -
Lecture notes
Suggested literature:

Title of the course: Research and Development in the pharmaceutical industry

Credit: 2

Coordinator /Department: Zsuzsa Majer, Department of Organic Chemistry

Terms for joining: BSc in chemistry (others: equivalent knowledge in organic chemistry)

Topics covered by the course:
The basic elements of Intellectual Property:
- The base lines of intelectual property and industrial property. Different protective forms.
- The Hungarian patent system and process. International patenting systems.
- Patents in chemistry and in pharmateutical industry.
- Industrial property information system, data bases.

Original drug research:
- Risks and expenses in the original drug research and development
- Targets of drug research, receptors
- Screening systems
- Features of the drug candidate for development

Compulsory literature*:

Suggested literature:
Lontai Endre: Szellemi alkotások joga (Eötvös József kiadó, Bp. 1998)
Szellemi tulajdonvédelemről mindenkinek (MIE 2002)
Önök kérdezték - iparjogvédelem, szerzői jog - mi válaszolunk (NSZH 2006)
Útmutató az iparjogvédelmi eljárásokhoz (MSZH 2006)
A szabadalmi bejelentés (MSZH 2004)
Drug Discovery Handbook (ed. S.C.Gad, John Wiley & Sons, 2005)

Title of the course: Ring transformations in heterocyclic chemistry

Credits:

Coordinator/Department: Antal Csámpai / Department of Inorganic Chemistry

Terms for joining: Successful exams:, Organic Chemistry, Organometallic Chemistry

Topics covered by the course: Systematic discussion and mechanistic interpretation of ring transformation of heterocyclic compounds with different ring size. The discussed conversions are distributed according to the synthetic methods using elektrophilic-, nucleophilic- dienophilic and dipolarophilic reagents, metal-containing catalysts and photolytic conditions. The syntheses of parent compounds with more complicated structures are also discused.

Literature*:
Compulsory:

Suggested:
H. C. Van der Plas: Ring transformation of heterocycles I-II. Academic Press, London and New York, 1973.

Title of the course: Structural bioinformatics

Credit: **2**

Coordinator /Department: Zoltán Gáspári / Department of Organic Chemistry

Terms for joining: Biochemistry

Topics covered by the course:
Primary and secondry databases in structural bioinformatics, quality assessment of experimentally determined macromolecular structures, domain recognition, secondary structure assignment, structure comparison and classification, contact-based approaches, idnetification of functionally important residues, introduction to structure prediction and the structure of nucleic acids

Compulsory literature:
The companion material accessible via WWW.

Suggested literature :
P.E. Bourne és H. Weissig (eds.): Structural Bioinformatics. Wiley-Liss, 2003.

Title of the course: Structure determination by spectroscopic methods

Credits: 2

Coordinator/Department: Antal Csámpai / Department of Inorganic Chemistry

Terms for joining: Solid knowledge of the basic concepts of IR, Raman, VCD, UV-VIS, UPS, CD and NMR spectroscopic methods and mass spectrometry.

Topics covered by the course:
Brief survey of the basic concepts of relevant spectroscopic methods indispensable for their practical applications. Solution of selected synthetic problems from organic, inorganic and metalloorganic chemistry through the structure elucidation of precursors, products and intermediates. This is based on the complementary information extracted from different spectra.. This practical course put special emphasis on the applications of multinuclear NMR techniques.

Literature*:
Compulsory:
Suggested:
J. T. Clerc, E. Pretsch and J. Seibl: Structural Analysis of Organic Compounds. Akadémiai Kiadó, Budapest, 1981
Faigl Ferenc, Kollár László, Kotschy András, Szepes László: Szerves fémvegyületek kémiája, Nemzeti Tankönyvkiadó, Budapest 2001
Sohár Pál: Mágneses magrezonancia spektroszkópia, Akadémiai Kiadó, Budapest, 1976.
Csámpai Antal, Jalsovszky István, Majer Zsuzsa, Orosz György, Rábai József, Ruff Ferenc, Sebestyén Ferenc: Szerves Kémiai Praktikum, Nemzeti Tankönyvkiadó, Budapest 1998.

Title of the course: **Structural investigation of proteins and peptides by spectroscopic methods**

Credits: **2 lectures / week, 2 credit**
Credit number: **2**
suggested lecture for every students having BSc

Coordinator: **Perczel András**

Department: **Organic Chemistry**

Closing the course: **colloquium**

Topics covered by this course:

The aim of this lecture is to provide both theoretical and practical aspects of the conformation analysis of organic- and bio-molecules and also to give the basics of spectral analysis and molecular modelling necessary for a structure oriented research. The primary goal of this course is to introduce the methodology of vibrational (FT-IR), electronic- (UV, CD) and nuclear magnetic (NMR) spectroscopy and also that of X-ray crystallography. Furthermore, the theoretical approximation of various levels of MM and QM theodes will be provided, especially covering the field of structure elucidation of proteins and peptides.

Compulsory literature: A. Perczel, I. Laczkó és M. Hollósi "*Peptidek térszerkezetvizsgálata* in A kémia újabb eredményei, 1994)
E-notes and handout of the lecture
Suggested literature: J.N.S.Evens *Biomolecular NMR Spectrscopy* (Oxford Univ. Press. 1995)
A.K.Downing *Protein NMR techniques* Sec.Edition (Humana Press 2004)

Title of the course: Structure – function of drugs I

Credit: 2
Coordinator/Department: Professor Ferenc Hudecz, Department of Organic Chemistry

Required pre-conditions: BSc in chemistry (others: equivalent knowledge in organic chemistry)

Topics covered by the course:

Quality, efficacy and safety aspects of drugs. Toxicology, genotoxicology and reproductive toxicology. Pharmacokinetics and drug-metabolism. Structure – function studies, experimental design. Stability studies. Mechanisms of action.
Interaction of drugs and other xenobiotics with the human body. Pharamacokinetics, phases of biotransformation.

Literature:
R. Ng: Drugs-From Discovery to Approval, Wiley, 2004
R. B. Silverman: The Organic Chemistry of Drug Design and Drug Action, Academic Press, 1992
P. Krogsgaard-Larsen, T. Liljefors and U. Madsen: Textbook of Drug Design and Discovery 3rd Edition, Taylor and Frances, 2002
Chi-Jen Lee *et al*.: Development and Evaluation of Drugs: From Laboratory through Licensure to Market, 2nd Edition, 2003
G. Thomas: Medicinal Chemistry: An Introduction, Wiley, 2001
J. Cannon: Pharmacology for Chemists (ACS Professional Reference Book), Oxford University Press, 1999

Title of the course: Structure – function of drugs II

Credit: 2
Coordinator/Department: Professor Ferenc Hudecz, Department of Organic Chemistry

Required pre-conditions: BSc in chemistry (others: equivalent knowledge in organic chemistry)

Topics covered by the course:

Cells and molecules of the immune system. Identification of B- and T- cell epitopes. Synthetic vaccines. Carcinogenesis, epidemiology, environmental effect. Diagnosis, tumour markers. radiotherapy, chemotherapy, immunotherapy. Combined therapy. Target molecules. Targeting of drugs, isotopes. Immunmodulation, immune suppression.
Classification and nomenclature of drugs. Metabolism, ADME properties. Targets of drugs, molecular mechanism of efficiency. Drugs affecting enzymes and receptors. Quantitative structure – function relationship.

Literature:
R. Ng: Drugs-From Discovery to Approval, Wiley, 2004
R. B. Silverman: The Organic Chemistry of Drug Design and Drug Action, Academic Press, 1992
P. Krogsgaard-Larsen, T. Liljefors and U. Madsen: Textbook of Drug Design and Discovery 3rd Edition, Taylor and Frances, 2002
Chi-Jen Lee *et al.*: Development and Evaluation of Drugs: From Laboratory through Licensure to Market, 2nd Edition, 2003
G. Thomas: Medicinal Chemistry: An Introduction, Wiley, 2001
J. Cannon: Pharmacology for Chemists (ACS Professional Reference Book), Oxford University Press, 1999

Title of the course: Synthesis and Characetrization of Liquid Crystals

Credit: 2

Coordinator/Department: István Jalsovszky, Dept. of Organic Chemistry

Lecturer: Katalin Fodor-Csorba, principal researcher,

Research Institute for Solid State Physics and Optics of Hungarian Academy of Sciences

Terms for joining:

MSc. Education in chemistry is needed. Basic knowledge of organic chemistry, physico-chemistry is necessary. (Sucessful exam of organic chemistry and physico-chemistry in BSc. at University of Eötvös Loránd is obligatory. (For other students equvivalent knowledge is important.)

Topics covered by the course:
Chemical architecture of liquid crystals, mesophase identification by optical polarizing microscopy and X-ray diffraction. Synthesis of deuterium labeled liquid crystals. Introduction to the investigation of the orientational order of liquid crystals by 2H NMR spectroscopy. Aromatic and heteroaromatic, alicyclic compounds and their synthesis. Chemical structure-mesophase property relations and their understanding. Molecular tayloring of ferroelectric materials. Liotropic systems. Polymeric liquid crystals. Comparation of the properties of linear and bent-core (banana-shaped) molecules, new mesophases. Electro-optical porperties of the materials for display techniques. Information storage by chemical way. Application of liquid crystals in the practice.

Suggested literature:

Bata Lajos: Folyadékkristályok Műszaki Könyvkiadó, Budapest, 1986.
B. Bahadur Liquid Crystals Application and uses Vol, I-III World Scientific. Singapore, 1991.
P. Collings, M. Hird: Introduction to Liquid Crystals, Taylor and Frances, 1998

Title of the course: Synthesis of biologically active peptides

Credit: 2

Coordinator /Department: Gábor Mező professor, HAS-ELTE Research Group of Peptide Chemistry

Terms for joining: requirements of the Chemistry Msc., basic knowledge in organic chemistry (successful exams in organic chemistry, for others: equivalent knowledge)

Topics covered by the course:
Introduction to the methods of peptide chemistry (synthesis in solution, solid phase peptide synthesis, ligation technics). Application of protecting groups, development of protecting scheme for successful synthesis. Side reactions under the synthesis and how they can be avoided. Advantages and drawbacks of the applied synthetic procedures. Planning of synthetic routes.

Compulsory literature*:
Medzihradszky Kálmán: A természetes peptidek szintézis. A kémia újabb eredményei 3 (1970)
Bajusz Sándor: Peptidszintézis. A kémia újabb eredményei 47 (1980)
G.A. Grant: Synthetic peptides, a user's guide (Freeman & Co., New York, 1992)

Title of the course: Theoretical approaches to protein science

Credits: 2+0

Coordinator/Department: Mónika Fuxreiter, Research fellow, HAS, Institute of Enzymology

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
Problems in structural biology, Modell construction, Force fields, Molecular mechanics, Molecular dynamics, Structural applications, MD analysis, Monte Carlo calculations for biomolecules, Biasing, protein structure prediction, Homology modelling, Electrostatics, Free energy calculations, pKa calcultions, simulation of enzymatic reactions, drug design

Literature*:
Compulsory: notes available on the internet

Suggested: Andrew Leach : Computer modelling
Arieh Warshel: Computer modelling of chemical reactions in enzymes and solutions

Name of the course: X-Ray Diffraction

Credit: 2

Coordinator /Department: Veronika Harmat research fellow/ Department of Organic Chemistry

Lecturers: Kálmán Simon, Veronika Harmat

Terms for joining: -

Topics covered by the course:

We discuss the bases of X-ray crystallography of small molecules and macromolecules.
1. Diffraction of X-rays
2. Theory of structure factors and Fourier synthesis
3. Symmetry of crystals and datasets
4. Direct methods
5. Structure refinement by least squares method
6. Crystallization and data collection
7. Solving the phase problem of macromolecular datasets
8. Density modification, model building
9. Refinement of macromolecular structures, maximum likelihood and molecular dynamics methods.
10. Crystallographic databanks

Suggested literature:

C. Giacovazzo, H.L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, G. Zanotti, M. Catti: „Fundamentals of Crystallography”, IUCr/Oxford University Press, 2002.

JP. Glusker, M. Lewis, M. Rossi: „Crystal Structure Analysis for Chemists and Biologists”, Whiley, 1994

Physical Chemistry - specialized module

Title of the course: Analysis of reaction mechanisms

Credits: 2 + 0

Coordinator/Department: Tamás Turányi, Physical chemistry

Terms for joining: Basic knowledge in physical chemistry

Topics covered by the course:
Development of reaction mechanisms in the traditional way and using computer codes, methods for the automatic generation of reaction mechanisms; local and global sensitivity analysis, interpretation of sensitivity coefficients, applications of sensitivity analysis; reduction of reaction mechanisms: identification of redundant species and reactions in a mechanism; time scale analysis: the quasi-steady-state approximation (QSSA), calculation of the error of the QSSA, the theory of slow manifolds (ILDM), the applications of ILDMs in chemical kinetics.

Literature*:
Compulsory: PowerPoint files on the Internet
Suggested:

A.S. Tomlin, T. Turányi, M.J. Pilling
Mathematical tools for the construction, investigation and reduction of combustion mechanisms
in: `Low temperature combustion and autoignition',
eds. M.J. Pilling and G. Hancock,
Elsevier, 1997, pp. 293-437

A. Saltelli ; K. Chan ; M. Scott (eds.)
Sensitivity Analysis.
Wiley, 2000 (ISBN: 0471998923)

A. Saltelli ; S. Tarantola ; F. Campolongo ; M. Ratto
Sensitivity Analysis in Practice: A Guide to Assessing Scientific Models
Wiley, 2004 (ISBN: 0-470-87093-1)

Title of the course: Analytical and numerical solution of chemical kinetics equations

Credits: 0 + 2

Coordinator/Department: István Lagzi, Physical chemistry

Terms for joining: Basic knowledge in physical chemistry and mathematics

Topics covered by the course:

Ordinary differential equation, existence and uniqueness of solutions, initial condition, phases plot, stationary points. Chemical kinetic equations, the system of ordinary differential equations, analytic method: separable equations, method of variation of parameters. n*th* order reaction, consecutive reaction, equilibrium reaction, autocatalytic, and oscillation reactions. Exact analytical solution of the chemical kinetics mechanisms, long-time behavior of solution. Basic of numerical methods: stability and convergence.

Literature*:

Compulsory: Notes on internet in progress

Suggested:

1. Scott, S. K. Oscillations, Waves and Chaos in Chemical Kinetics, Oxford University Press, Oxford, (1995).
2. Epstein, I. R.; Pojman, J. A. An Introduction to Nonlinear Chemical Dynamics, Oxford University Press, New York, (1998).

Title of the course: Applications of polyelectrolyte/surfactant systems

Credits: 2

Coordinator/Department: Róbert Mészáros, Physical chemistry

Terms for joining: Basic knowledge in physical and/or colloid chemistry

Topics covered by the course:
Polyelectrolyte/surfactant interaction
The mechanism of polyelectrolyte/surfactant interaction and the cooperativity of surfactant binding. Biomacromolecule/surfactant interaction and its physiological effects.
Phase properties of polyelectrolyte/surfactant mixtures
Phase diagrams of the aqueous mixtures of oppositely charged macromolecules and amphiphiles and their correct representation.
Industrial applications
The role of the interfacial behaviour of polyelectrolyte/surfactant mixtures in the development of next generation products for the cosmetics and household care industry.

Literature*:
Compulsory: Notes on internet in progress
Suggested:
1. Claesson P.M, Dedinaite A., Mészáros R., Varga I.: *Association between polyelectrolytes and oppositely charged surfactants in bulk and at solid/liquid interfaces*, Colloid Stability and Application in Pharmacy: Volume 3, Editor Tharwat Tadros, Wiley, 2007 ISBN: 978-3-527-31463-8
2. Radeva, T.: *Physical Chemistry of Polyelectrolytes,* In Surfactant Science Series;. Marcell Dekker Inc.: New York, 2001
3. Wei, Y.C.; Hudson, S.M : *The interaction between polyelectrolytes and surfactants of opposite charge* J. Macromol. Sci. Rev. Macromol. Chem. Phys. C35, 15, 1995
4. Mészáros R., Thompson L., Bos M., Varga I., Gilányi T.: *Interaction of sodium dodecyl sulfate with polyethyleneimine: Surfactant induced polymer solution colloid dispersion transition* Langmuir 19, 609-615, 2003

Title of the course: Applied computer simulations

Credits: 2

Coordinator/Department: László Túri, Department of Physical Chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
The purpose of the course is to introduce the basic computer simulation methods applied in the research of the atomic and molecular structure, and dynamics of liquids. We briefly outline the theoretical basis of selected techniques, discuss the possible solutions of their numerical problems, and illustrate the applicability of the methods.

Classical mechanics part: Introduction to classical mechanics and classical statistical mechanics, Monte Carle technique, molecular dynamics, evaluation of MC and MD simulations, non-equilibrium molecular dynamics, experimental connections and implications.
Quantum mechanical part: Born-Oppenheimer dynamics, Car-Parrinello dynamics, semi-classical simulations, path-integral methods.

Compulsory*:
Lecture notes on the internet (in preparation)
Suggested:
M. P. Allen, D. J. Tildesley, Computer Simulation of Liquids, Oxford University Press, 2003
J. M. Thijssen, Computational Physics, Cambridge University Press, 2000
D. Marx, és J. Hütter, Ab Initio Molecular Dynamics: Theory and Implementation (Modern Methods and Algorithms of Qunatum Chemistry, szerkesztő: J. Grotendorst, John von Neumann Institute for Computing, Jülich, 1. kötet, 301-449, 2000)

Title of the course: Applied Colloid Science

Credits: 1 + 3

Coordinator/Department: Ferenc Csempesz, Physical Chemistry

Terms for joining: Basic knowledge in physical and colloid chemistry

Topics covered by the course:

Colloid particles, basic principles of formation and elimination of colloid systems. Disperse and cohesive systems of colloids, natural nano-size structures. Colloids in bio-medical, pharmaceutical, agricultural, industrial and environmental applications. Colloids and colloid-physical/chemical methods for controlling kinetic stability, electrokinetic and transport processes and rheological properties.

Literature*:

Compulsory:
Wolfram E.: Kolloidika (lecture notes), II/2 és I-III választott részek, Tankönyvkiadó, Budapest, 1977
Rohrsetzer S.: Kolloidika (book), választott részek, Tankönyvkiadó, Budapest, 1991

Suggested:
Gábor M.: Az Élelmiszer előálítás kolloidikai alapjai, (book) Mezőgazdasági Kiadó, Budapest 1987
J. Kreuter: Colloidal Drug Delivery Systems, Marcel Dekker Inc., New York, 1994
K. Holmberg: Handbook of Applied Surface and Colloid Chemistry, Vol.:1,2, Wiley&Sons, England, 2001. ISBN 0-471-49083-0

Title of the course: Biocompatible surfaces

Credits: 2

Coordinator/Department: Kiss, Éva, associate professor Department of Physical Chemistry

Terms for joining: beginning terms of the Chemistry MSc., basic knowledge in colloid and surface chemistry (for those having an ELTE chemistry Bsc.: Basics of Colloid and Surface Chemistry, KA2KL1 and KA2KL2; for others: equivalent knowledge)

Topics covered by the course:

The biocompatibility and its relation to the application of biomaterials. Polymeric biomaterials, the dynamics of polymer surfaces. The analysis of the „bio response” as an interfacial phenomenon.

Concepts of surface modification and design. Experimental techniques to characterize the interaction between biomaterials and bioliquids. The role of protein adsorption, its characteristic features and possible investigation.

Practical examples: implants, medical devices, drug delivery systems.

Literature*:

Compulsory:

J. D. Andrade: Surface and Interfacial Aspects of Biomedical Polymers, Plenum Pr. N.Y. 1985. B. D. Ratner, A. S. Hoffman, F. J. Schoen, J. E. Lemons: Biomaterials Science, Academic Pr. San Diego, 1996.

Suggested:

Kiss Éva: Kardiovaszkuláris anyagok. Műszaki felülettudomány és orvosbiológiai alkalmazásai. (Szerk: Bertóti Imre, Marosi György, Tóth András) B+V Kiadó, Budapest, 2003. pp 260-277.

Scientific papers in Medical Devices

Title of the course: Bulk and surface interaction between macromolecules and surfactants

Credits: 2

Coordinator/Department: Róbert Mészáros, Physical chemistry

Terms for joining: Basic knowledge in physical and/or colloid chemistry

Topics covered by the course:

Interaction between neutral polymers and amphiphile molecules

Description of surfactant self assemblies. Thermodynamic models of polymer/surfactant complexes. The effect of different parameters (such as the surfactant concentration as well as the structure, size and chemistry of macromolecules) on the nature of the polymer/surfactant complexes.

Interfacial layers of macromolecules and surfactants

Adsorbed layers formed from the solutions of polymers and surfactants. Surface modification of polymer coated solid surfaces in the presence of surfactant solutions. The interrelation between the structure of interfacial macromolecule/surfactant complexes and the nature of bulk polymer/surfactant aggregates.

Literature*:

Compulsory: Notes on internet in progress

Suggested:

1. Goddard, E. D.: *Interactions of Surfactants with Polymers and Proteins*;, Ananthapadmanabhan, K. P., Eds.; CRC Press: Boca Raton, FL, 1993

2. Kwak, J.C.T. *Polymer-Surfactant Systems*;, Ed.; Surfactant Sci. Ser.; Marcel Dekker: New York, 1998

3. K, Holmberg, B. Jönsson, B. Kronberg, Lindman B.: *Surfactants and Polymers in Aqueous Solution* John Wiley & Sons; 2.ed., 2002

4. Hansson, P.; Lindman, B.: *"Surfactant-polymer interactions"* Curr. Opin. Colloid Interface Sci. 1, 604-613, 1996

5. Mészáros R, Varga I, T.Gilányi T
Effect of Polymer Molecular Weight on the Polymer/Surfactant Interaction
J. Phys. Chem. B. 2005, 109, 13538-13544

Title of the course: Chemical dynamics in liquid phase

Credits: 2

Coordinator/Department: László Túri, Department of Physical Chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
The course provides a consistent discussion of the molecular dynamics of liquid phase molecular events and chemical reactions.

Theoretical basics: classical and quantum dynamics, classical and quantum electrodynamics
Liquids, solids, interfaces
Methods: time-correlation functions, stochastic processes, relaxation processes
Quantum statistical mechanics, density operator
Linear response theory
Applications: vibrational relaxation, electron transfer reactions, spectroscopy

Compulsory*:
Lecture notes on the internet (in preparation)
Suggested:
A. Nitzan, Chemical Dynamics in Condensed Phases; Relaxation, Transfer and Reactions in Condensed Molecular Systems, Oxford University Press, 2006
V. May és O. Kühn, Charge and Energy Transfer Dynamics in Molecular Systems, Wiley, Weinheim, 2004
C. Cohen-Tannoudji, B. Liu és F. Laloë, Quantum Mechanics, Wiley, New York, 1977

Title of the course: Chemometrics

Credits: 2+0

Coordinator/Department: Gergely Tóth, Dept. of Physical Chemistry

Terms for joining: Standard Course in Mathematics for BSc Students in Chemistry

Topics covered by the course:
Chemometrics means multivariate statistics applied to Chemistry. The course includes (a) exploratory statistics (handling, preprocessing and visualisation of categorical and metric data, supervised and unsupervised pattern recognition (clustering, classification), rediction of dimension (principal componnent analysis), (b) parametric statistics (linear and nonlinear regression, statistics of parameters, estimated and predicted responses. Diagnostics of regression, Solving ill conditioned regression problems, ridge-, principal component- and partial least squares regression. Soft modeling. Robust parameter estimation.

Literature*:
Compulsory:
I. Frank, R. Todeschini: Data Analysis Handbook. (Elsevier, 1994)
Füstös,L – Meszéna,G. -Simonné Mosolygó D.: A sokváltozós adatelemzés matematikai módszerei (Akadémiai Kiadó)
Suggested:
G.A.Korn-T.M.Korn: Mathematical Handbook for Scientists and Engineers. (McGraw Hill)
Horvai G. (ed): Sokváltozós adatemelemzés (kemometria).Nemzeti Tankönyvkiadó, 2001.
+ SCAN, Origin, MATLAB, EXCEL programming manuals,

Title of the course: Computational Chemistry

Credits: 2

Coordinator/Department: Fogarasi, Geza / Inorganic Chemistry

Terms for joining: at least two semesters of physical chemistry and one semester of theoretical chemistry

Topics covered by the course:
Molecular mechanics: theoretical basis, fields of applications, assessment of limitations. Electronic structure of molecules: an overview of methods of quantum chemistry; practical aspects: basis sets, treatment of electron correlation; semiempirical methods; density functional theory (DFT). Structural research by computational methods. Symmetry and molecular structure, with a brief introduction to group theory. Studying chemical reactions: transition state theory and statistical mechanics; reaction mechanisms, qualitative theories. Computer simulation of dynamic phenomena.

Literature*:

Compulsory:

1. Frank Jensen: Introduction to Computational Chemistry, John Wiley & Sons, Chichester, New York; 1999. ISBN: 0 471 98425 6.

Suggested:

2. Christopher J. Cramer: Essentials of Computational Chemistry, John Wiley & Sons, Chichester, 2002. ISBN: 0 471 48552 7.
3. Errol Lewars: Computational Chemistry, Kluwer Academic, Boston/Dordrecht/London, 2003. ISBN: 1-4020-7285-6.

Title of the course: Computational methods for electronic structure

Credits: 2 + 0

Coordinator/Department: Prof. Péter Szalay, Physical Chemistry

Terms for joining: Electronic structures of molecules

Topics covered by the course:
This course provides the basic knowledge of theoretical methods and procedures which can be used to describe the electronic structure of molecules. Both ab initio and and DFT methods will be discussed. The main goal is to demonstrate the the applicability and limits of these widely used methods.

Literature*:
Compulsory: Notes on internet in progress
Attila Szabo és Neil S. Oslund: Modern Quantum Chemistry, Dover Publications, 1996
Suggested:

Title of the course: Computer-driven experiments

Credits: 0+2
Coordinator, department: Ernő Keszei, Physical Chemistry

Prerequisits: B.Sc. courses in physical chemistry

Topics of the course:

Topics covered: Experiments and measurements using scientific instruments. Process control. Operational model of a desktop computer. Communication of a computer with external devices. Modular assembly of computer-driven experimental setups. Interfaces. Using the i8255 interface. Data collection and storage using USB, printer and serial ports. A/D and D/A converters. Sensors and their transfer functions. Transforming non-electrical signals to electric signals. Characterisation of some actual computer-driven experimental setups.
Practical work: Data collection using a PC. Determination of transfer functions. Writing a computer code to control an experiment.

Textbooks to use

Compulsory: R. P. Wayne: Chemical Instrumentation, Oxford University Press: 1994.
R. W. Cattral: Chemical Sensors, Oxford University Press: 1997.

Recommended: Szalma J., Láng Gy., Péter L.: Alapvető fizikai kémiai mérések és a kísérleti adatok feldolgozása, Eötvös Kiadó 2007 (in Hungarian)

Title of the course: Computer techniques

Credits: 1

Coordinator: KUZMANN, Ernő

Department: Department of Analytical Chemistry

Prerequisites: Basic mathematics high school knowledge

Topics covered by the course:
Development of computer technique. Computer generations. Basics of computer techniques. Basics of Boole algebra. Logical functions, Karnough tables. Electronic circuits, AND, OR, NOT, NAND. Multivibratores, scalers, memories. Logical structures of personnel computers. Computer codes, registers, commands. DOS and WINDOWS operation systems. Basics of FORTRAN language. Basics of PASCAL language.

Literature:
Gyula Löcs and József Vigassy, FORTRAN computer language, Mûszaki Könyvkiadó, Budapest, 1985 (in Hungarian)
Erzsébet Gordon, Gézáné Körtvélyesi, István Sós, Zoltán Székely, PASCAL computer language, SZÁMALK, Bp. 1982. (in Hungarian)

Title of the course: Computer technique practice

Credits: 3

Coordinator: KUZMANN, Ernő

Department: Department of Analytical Chemistry

Prerequisites: Basic mathematics high school knowledge. The course is connected to the lecture.

Topics covered by the course:
Computer codes, commands. Use of DOS and WINDOWS operation systems. Programs in FORTRAN language. Programs in PASCAL language.

Literature:
Gyula Löcs and József Vigassy, FORTRAN computer language, Mûszaki Könyvkiadó, Budapest, 1985 (in Hungarian)
Erzsébet Gordon, Gézáné Körtvélyesi, István Sós, Zoltán Székely, PASCAL computer language, SZÁMALK, Bp. 1982. (in Hungarian)

Title of the course: Corrosion and electrodeposition of metals

Credits: 2

Coordinator/Department Laura Sziráki, associate professor, Physical chemistry

Terms for joining: physical chemistry (successful exams of BSc courses)

Topics covered by the course:
The course is focused on the a) physical-chemical fundamentals of the environmental reactions of metals , b) measurement and control techniques of the corrosion of metals, alloys, and structural materials , c) fundamentals in theory and practice of the conventional and novel industrial electrodeposition techniques with emphasis on their environmental hazards and protective values. The corrosion rate measurement and electrodeposition techniques are demonstrated on laboratory practices.

Literature*:
Compulsory: lecture notes (on internet in progress), selected papers
Laboratory practices on environmental analysis and environmental technology, Eds. Enikő Varga, Tibor Garai Ch. X-XIII, pp. 223-294, ELTE Eötvös Publ., Budapest 1999.
Suggested
J. Dévay: Corrosion and corrosion protection of metals, Műszaki Publ., Budapest, 1979
L. Kiss: Introduction of electrochemistry, university textbook, 1997
J. Dévay: Passivity, crevice corrosion, pitting corrosion; Stress corrosion of metals, Akadémia Publ., 1979, Series of new results in chemistry Vol. 44.

Title of the course: Disorder in condensed phases

Credits: 2

Coordinator/Department: László Pusztai, RISSPO HAS/Physical chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
The lectures will introduce basic concepts/functions/quantities applicable for describing structural disorder in the liquid and solid (amorphous and crystalline) phases. Most of the time will be spent on discussing (primarily, experimental) methods available for determining these functions/quantities.
The structure factor and the pair correlation function. Higher order correlations.
Determination of the structure factor using diffraction methods.
Experimental techniques based on X-ray absorption.
Computer (molecular dynamics and Monte Carlo) simulations. Methods for 'direct' structural modelling.
Liquid structures. The structure of metallic and covalent glasses. Disorder in crystals.

Literature*:
Compulsory: Notes taken during the lectures; web-based outline will also be available.
Suggested: M.T. Dove: Structure and Dynamics (Oxford University Press, 2003)
V.M. Nield, D.A. Keen: Diffuse neutron scattering from crystalline materials (Clarendon Press, Oxford, 2001)
Kémia újabb eredményei 80. kötet, Akadémiai, 1995.

Title of the course: Electrostatic interactions in colloid systems

Credits: 2

Coordinator/Department: Tibor Gilányi, Physical chemistry

Terms for joining: Basic knowledge in colloid and surface chemistry

Topics covered by the course:
Electric structure of interfaces. Helmholtz model. Gouy-Chapman theory. Discrete and continous descriptions of the interfaces.
Electrokinetic phenomena. Theory of the zeta-potencial.
Problematics of pH determinations in colloid and biological systems. The suspension potencial. Different interpretations of the Donnan equilibrium. Adsorption of ions. Adsorption isotherm equations.
Interactions in ionic micellar systems, micelle formation, mixed micelle formation, polymer-surfactant complexes.

Literature*:
Suggested
R. J. Hunter: Foundation of Colloid Science, Clarendron Press, Oxford, 1993

Title of the course: Elementary reaction dynamics

Credits: 2

Coordinator/Department: László Túri, Department of Physical Chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
The course discusses elementary aspects of chemical reactions, providing a connection of the molecular basics of chemical reactions to the experimentally measurable kinetic quantities.

Reactive and non-reactive dynamics
Classical and quantum mechanical scattering theory
Reactive dynamics: approximations to molecular dynamics methods, potential surfaces, chemical reactions
Rate of chemical reactions, rate constants
Adiabatic and non-adiabatic reaction dynamics
Non-reactive dynamics: introduction to the dynamics of transfer processes

Compulsory*:
Lecture notes on the internet (in preparation)
Suggested:
R. D. Levine és R. B. Bernstein, Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, 1987
V. May és O. Kühn, Charge and Energy Transfer Dynamics in Molecular Systems, Wiley, Weinheim, 2004
C. Cohen-Tannoudji, B. Liu és F. Laloë, Quantum Mechanics, Wiley, New York, 1977

Title of the course: Exploration of reaction mechanism with theoretical methods

Credits: 2 +0

Coordinator/Department: András Stirling, Chemical Research Center

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
Exploration of potential energy surface: quantum chemical methods; important regions; transition state searching methods; entropy information, surface crossing.
Exploration of free energy surface: ensembles; quantum chemical methods; transition state searching methods for non-zero temperature;

Literature*:
Suggested: F. Jensen: Introduction of Computational Chemistry; D. Frenkel, B. Smit: Understanding Molecular Simulation

Title of the course: Femtochemistry

Credits: 2
Coordinator: Keszei, Ernő

Department: Physical Chemistry

Prerequisits: B.Sc. courses in physical chemistry

Topics of the course:

Introductory topics: What is femtochemistry? Outline of the history of kinetics concerning time resolution and theories. Lasers, laser photolysis. Timescale in chemistry, especially in the 10^{-18} - 10^{-10} s domain. Specific problems in ultrafast laser pulse treatment.
Elements of nonlinear optics: Basics of geometrical optics: mirrors, lenses, prisms, filaments. Wave optics: wave equations and their solutions for optical devices. Vector optics, polarization. Nonlinear optical phenomena: second and higher harmonics, self-phase modulation, self-focalisation, optical parametric amplifiers, Kerr lenses. Optical description of Gaussian beams. Lasers, pulsed lasers, semiconductor lasers, photodetectors. Generation and amplification of ultrafast laser pulses.
Topics of femtochemistry: Spectral and temporal characteristics of laser pulses. Transform-limited pulses. Experiments using two and three laser pulses. Quantitative treatment of pump-probe measurements. Convolution in femtochemical detection. Deconvolution methods. Experimental study of unimolecular reactions using pump-probe techniques. Reconstruction of interatomic potentials. Studying molecular anisotropy. Initialising coherent bimolecular reactions using pump-probe techniques.

Textbooks to use

Compulsory: J. Manz, L. Wöste (editors): Femtosecond Chemistry 1-2, WCH Weinheim, 1995
E. Keszei: Femtokémia: a pikoszekundumnál rövidebb reakciók kinetikája, Akadémiai Kiadó Budapest, 1999 (in Hungarian)

Recommended: B. A. Saleh, M. C. Teich: Fundamentals of Photonics, John Wiley & Sons

Title of the course: Interfacial Behaviour of Macromolecules

Credits: 2 + 0

Coordinator/Department: Ferenc Csempesz, Physical Chemistry

Terms for joining: Basic knowledge in physical and colloid chemistry

Topics covered by the course:

Macromolecular solutions. Dissolved macromolecules at interfaces: thermodynamic and kinetic aspects of polymer adsorption. Equilibrium adsorption: excess quantities, adsorption isotherms. Polymer adsorption theories. Structure of interfacial polymer layers, conformation of adsorbed macromolecules, steric interactions. Competitive adsorption of macromolecules from polymer mixtures. Characterization of preferential adsorption.

Literature*:

Compulsory:
Wolfram E.: Kolloidika (lecture notes), II/2 és I-III választott részek, Tankönyvkiadó, Budapest, 1977
Rohrsetzer S.: Kolloidika (book), választott részek, Tankönyvkiadó, Budapest, 1991

Suggested:
G.J. Fleer et al.: Polymers at Interfaces, Chapman & Hall, London, 1993.
Bárány S.,:Polimerek diszperz rendszerekben,(book) Akadémiai Kiadó, Budapest, 2000.

Title of the course: Introduction to chemical thermodynamics

Credits: 2
Coordinator Department: Ernő Keszei, Physical Chemistry

Prerequisits: B.Sc. calculus courses and physics courses

Topics of the course:

Outline of basic thermodynamics: History and conceptually different foundations of thermodynamics. Postulatory thermodynamics: simple systems and postulates. Equilibria in isolated and adiabatic systems. Fundamental equations and equations of state. Equilibria at constant pressure, temperature, and when both are constant. Thermodynamic potentials and their interrelations. Thermodynamic functions in terms of measurable quantities.
Chemical thermodynamics: What is physical chemistry? Thermodynamics in systems of multiple components. Chemical potential in ideal and real mixtures. Absolute and relative activity. Phase equilibria of pure substances. Phase equilibria in binary systems: binary liquid-vapour, liquid-liquid and solid-liquid phase diagrams. The partition coefficient. Colligative properties: vapour pressure reduction, boiling point elevation, freezing point depression, osmosis, porous diffusion. Phase equilibria in multiple component systems. Thermodynamic description of chemical reactions in ideal and real solutions. Temperature and pressure dependence of the equilibrium constant. Application of the Le Chatelier-Braun principle. Systems containing electrically charged particles. The electroneutrality principle and its consequences in thermodynamics. The electrochemical potential. The thermodynamic nature of charge carriers and electric conduction. Heterogeneous electrochemical equilibria. Galvanic cells and electrodes. The p_H electrode.

Textbooks to use

Compulsory: P. W. Atkins: Physical Chemistry, Oxford University Press, 2005

Recommended: H.B. Callen: Thermodynamics, an Advanced Treatment for Chemists and Physicists, New York, 1985
E. A. Guggenheim: Thermodynamics and an Introduction to Thermostatistics, Amsterdam, 1950
E. Keszei: Bevezetés a kémiai termodinamikába
(lecture notes in Hungarian to be published)

Title of the course: Investigation methods in materials science A: atomic scale

Credits: 2

Coordinator/Department: Kiss, Éva, associate professor Department of Physical Chemistry

Terms for joining: beginning terms of the Chemistry MSc., basic knowledge in physical, colloid and surface chemistry

Topics covered by the course:

Overview of the calculation and modelling methods. Infrared and RAMAN spectroscopy (polymers, ceramics and composite materials).
NMR spectroscopy (solid samples, crystals, multinuclear characterization of gels and amorf materials).
Mass spectrometry (small and large molecules, polymers, biomolecules, metals and alloys).
Nuclear techniques: Mössbauer spectroscopy (phase analysis of alloys, application for coordination chemistry, biological systems) and positron annihilation (relation between annihilation parameters and materials structure, thermalization of the positron, measuring techniques)

Literature*:
Compulsory:
Kiss É. A kémia újabb eredményei, 95. Akadémiai Kiadó, Budapest, 2006.
Suggested:
J. Frommer, R.M. Overney, Interfacial Properties on the Submicrometer Scale, Am. Chem. Soc., Washington, 2000.
C.N.R. Rao, A. Müller, A.K. Cheetham, The Chemistry of Nanomaterials, Wiley-VCH Verlag, Weinheim, 2004.

Title of the course: Lasers in chemistry

Credits: 2

Coordinator/Department: Inorganic Chemistry

Terms for joining:

Topics covered by the course:
1. Introduction, invention and history of lasers
2. Basic physics of lasers
3. Laser sources
4. Manipulation of the laser beam
5. Laser spectroscopy: methods and applications
6. Laser spectroscopy in analytical chemistry, LIDAR
7. Photochemistry, laser stimulated and sensitized reactions
8. Ultrafast kinetic measurements
9. Selected non-chemical applications of lasers: holography, laser cooling of atoms, photoassociation spectroscopy, atomic clocks; astronomical masers and lasers

Literature*:
Compulsory: -

Suggested:
Anthony E. Siegman: Lasers, University Science Books, 1986.
William T. Silfvast: Laser Fundamentals, Cambridge University Press, 2nd ed. 2004.
David L. Andrews: Lasers in Chemistry, Springer, 1997.
Halina Abramczyk: Introduction to Laser Spectroscopy, Elsevier, 2005.
Gerald R. Van Hecke and Kerry K. Karakstis: A Guide to Lasers in Chemistry, Jones and Bartlett Publishers, 1998.
Anne B. Myers, Thomas R. Rizzo (Editors): Laser Techniques in Chemistry, Wiley, 1995.
Ahmed H. Zewail: Laser Chemistry Applications, (Photochemistry and Photobiology, Vol.1.), Gordon & Breach Publishing Group, 1983.

Title of the course: Mass Spectrometry

Credits: 2

Coordinator/Department: Károly Vékey, Chemical Research Center, HAS

Dávid Frigyes, Dept. of Inorganic Chemistry

Terms for joining:

Basic Knowledge in physical and organic chemistry

Topics covered by the course:
The aim of the course is to introduce the students into mass spectrometry, one of the most important methods in analytical chemistry. 1) Basics of mass spectrometry: instrumentation, classical applications. 2) Modern mass spectrometry: most important new developments and methods. Emphasis is given on ionization methods (electrospray, MALDI), GC–MS, HPLC–MS, tandem MS. 3) Application of mass spectrometry in diverse fields, including organic, bioorganic pharmaceutical applications, proteomics, food and environmental analysis, medical diagnostics, materials science

Literature:
Compulsory: lecture notes

Suggested:

Name of Course: Mass Spectrometry : Operation of mass spectrometers.

Credit: 2

Coordinator /Department: Dr. László Bencze, Institute of Chemistry, Dept. of Physical Chemistry

Terms for joining: requirements of the Chemistry MSc., basic knowledge in physics, mathematics and physical chemistry (Chemistry BSc).

Topics covered by the course:
History of mass spectrometry. Construction of mass spectrometers. Types of ion sources. Types of mass analysers. Single focusing: direction focusing and velocity focusing. Double focusing. Scanning methods. Linked scans and their application in the research of structure. Detectors. Vacuum system of mass spectrometers. Sampling systems.

Compulsory literature:
Slides about the lecture.
Suggested literature:
Kaposi Olivér: Tömegspektrometria I., Tankönyvkiadó. Budapest, 1989 (Hung.).
A kémia újabb eredményei 45. kötet, Akadémiai Kiadó, Budapest, 1979 (Humg.).
Cornides István: Gyakorlati tömegspektroszkópia, Műszaki Könyvkiadó, Budapest, 1970 (Hung.).
Simonyi Károly: Elektronfizika (Hung.).
Kelman-Javor: Elektronoptika, Akadémiai Kiadó, Budapest, 1965 (Hung. translation).

Title of the course: Metastable liquids

Credits: 2

Coordinator/Department: Attila Imre, KFKI Atomic Energy Research Institute

Terms for joining: Basic knowledge (BSc) in physical chemistry

Topics covered by the course:
- Stability limits; metastability in thermodynamics and in statistical physics.
- Physical chemistry of liquids under negative pressure.
- Experimental technics.
- Liquids under negative pressure in biology and in Earth sciences.
- Glasses and supercooled materials.

Literature*:
Compulsory:
Lecture notes.
Suggested:
- P.G. Debenedetti: Metastable Liquids: Concepts and Principles, Princeton University Press, Princeton, NJ, 1996
- A. Imre, K. Martinás and L.P.N. Rebelo: Thermodynamics of Negative Pressures in Liquids, Journal of Non-Equilibrium Thermodynamics, vol.23, pp351-375, 1998
- Liquids Under Negative Pressure (Eds.: A.R. Imre, H.J. Maris and P.R. Williams) NATO Science Series, Kluwer, Dordrecht, 2002

Title of the course: Modern surface analytical techniques in electrochemistry

Credits: 2 + 0

Coordinator/Department: Gabor Nagy, Physical chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:

The aim of the course is to introduce those surface analytical techniques which are capable to investigate the atomistic properties of solid/liquid interfaces
The following methods are presented: canning tunneling microscopy, atomic force microscopy, infra-red spectroscopy, synchrotron X-ray diffraction, and some other scanning techniques
Theoretical foundations, realization and interesting results are discussed.

Literature*:
Compulsory: lecture notes
Suggested:

A.J. Bard – L. Faulkner: Electrochemical Methods, Fundamentals and Applications
P.W. Atkins: Physical Chemistry
H.D. Abruna: Electrochemical Interfaces, VCH 1991

Title of the course: New chemical methods in materials science B

Credits: 2

Coordinator/Department: Kiss, Éva, associate professor Department of Physical Chemistry

Terms for joining: beginning terms of the Chemistry MSc., basic knowledge in physical, colloid and surface chemistry

Topics covered by the course:

Preparation and stability of nanodisperse systems, spontaneously formed nanosystems. Nanocomplexes and nanoparticles of polymers with surface active agents. Preparation of polymeric responsive nanosystems in bulk and at interfaces. Controlling of interfacial properties by macromolecules.
Preparation and application of conductive polymers.
Chemical vapour deposition. Surface modification by electrochemical methods.
Ordered molecular nanolayers. Self assembled, Langmuir and Langmuir-Blodgett films.

Literature*:
Compulsory:
Kiss É. A kémia újabb eredményei, 95. Akadémiai Kiadó, Budapest, 2006.
Suggested:
J. Frommer, R.M. Overney, Interfacial Properties on the Submicrometer Scale, Am. Chem. Soc., Washington, 2000.
C.N.R. Rao, A. Müller, A.K. Cheetham, The Chemistry of Nanomaterials, Wiley-VCH Verlag, Weinheim, 2004.

Title of the course: Numerical methods in chemistry - lecture

Credits: 2+0

Coordinator/Department: Attila Császár, Department of Physical Chemistry

Terms for joining: Basic knowledge in mathematics

Topics covered by the course:
Selected numerical methods and their application in chemistry:
Linear equations, Ordering, Random numbers, Non-linear set of equations, Roots of polynomials, Search for minima and maxima, Numerical differentiates, integrals, interpolation techniques, Parameter fitting, Eigenvalues, Differential equations, Fourier transformation, Search for global minima, Neural networks, Principal component analysis

Literature*:
Compulsory Attila Császár - Gergely Tóth: lecture notes.
Suggested:
C. Lanczos: Numerical Analysis, Dover: New York, 1976.
Valkó P. és Vajda S.: Műszaki–tudományos feladatok megoldása személyi számítógéppel, Műszaki, 1987.
Horvai (ed): Sokváltozós adatelemzés (kemometria),

Title of the course: Numerical methods in chemistry - practice

Credits: 0+2

Coordinator/Department: Gergely Tóth, Department of Physical Chemistry

Terms for joining: Parallel completion of the lecture

Topics covered by the course:
Programming in C or Fortran for chemical problems in the topics of:
Linear equations, Ordering, Random numbers, Non-linear set of equations, Roots of polynomials, Search for minima and maxima, Numerical differentiates, integrals, interpolation techniques, Parameter fitting, Eigenvalues, Differential equations, Fourier transformation, Search for global minima, Neural networks, Principal component analysis

Literature*:
Compulsory Attila Császár - Gergely Tóth: lecture notes.
*Suggested***:**
C. Lanczos: Numerical Analysis, Dover: New York, 1976.
Valkó P. és Vajda S.: Műszaki–tudományos feladatok megoldása személyi számítógéppel, Műszaki, 1987.
Horvai (ed): Sokváltozós adatelemzés (kemometria),

Title of the course: Photophysical and Photochemical Kinetics

Credits: 2

Coordinator/Department: Attila Demeter, IMEC CRC HAS,

Terms for joining: Basic courses of chemistry from physical and organic chemistry

Topics covered by the course:
The basic concepts and ideas of reaction kinetics and photochemistry.
The role and nature of the radiative and nonradiative processes. Energy transfer reactions. Methods of preparative photochemistry, kinetics studies, and data handling. The dual luminescence phenomenon: an example of the photophysical kinetics examinations. Photoreduction: kinetics of the primary and secondary reactions. Electron transfer reactions: the Marcus theory. Eximers and exciplexes: spectroscopy and kinetics. Solvent effect and hydrogen bonding. The influence of the diffusion controlled reactions on the kinetics. Conservation of the orbital symmetry: photocycloaddition and pericyclic reactions. Photoelimination and the Norrris I and II reactions, the properties of biradicals; photochemistry of transient species. Photo-oxidation, chemiluminescence and the photochemical smog phenomenon. Biological and practical concern of photochemistry.

Literature*:
Compulsory: The material of the seminar in .ppt file.
Suggested: **http://www.chemres.hu/scientists/demeter/kandiv.pdf** **(hun.)**
http://www.chemres.hu/scientists/demeter/disszertacio.pdf **(hun.)**
Horvát Attila: Szervetlen Fotokémia (VE Kiadó) bevezető fejezetei. (**hun.)**
J.R.Lakowicz: Principles of Fluorescence Spectroscopy, Plenum Press, NY 1983.
A. Gilbert, J. Bagott: Essential of Molecular Photochemistry, Blackwell, Oxford, 1991.

Title of the course: Physical Stability Colloidal Drug Carriers

Credits: 2 + 0

Coordinator/Department: Ferenc Csempesz, Physical Chemistry

Terms for joining: Basic knowledge in physical and colloid chemistry

Topics covered by the course:

Colloid particles, basic principles of formation and elimination of colloid systems. Colloidal disperse and cohesive systems. Nano-size structures in living organizations. Stability and stabilization of colloids in pharmaceutical preparations. Utilization of colloids for controlling surface and electrokinetic properties of particles. Kinetic stability and rheological properties of pharmaceutical dispersions.

Literature*:

Compulsory:

Rohrsetzer S.: Kolloidika (book), választott részek, Tankönyvkiadó, Budapest, 1991
Rácz I., Selmeczi B.: Gyógyszer technológia I-III (book), választott részek, Medicina, Budapest, 2001

Suggested:

J. Kreuter: Colloidal Drug Delivery Systems, Marcel Dekker Inc., New York, 1994
R. H. Müller: Colloidal Carriers for Controlled Drug Delivery and Targeting, Wissenschaftliche Verlagsgesselschaft mbH, Stuggart, 1991

Title of the course: Practical work in chemical informatics A and B

Credits: 0 + 4

Coordinator/Department: Tamás Turányi, Physical chemistry

Terms for joining: Basic knowledge in physical chemistry

Topics covered by the course:
During the practice, a chemical problem is solved using a high-level programming language or environment (*e.g.* pl. Fortran, Pascal, C, C++, LabVIEW, MATLAB, Mathematica). The chemical problems investigated include data acquisition, molecular modelling, theoretical chemistry, reaction kinetics. The aim is a good quality solution of a real problem based on individual efforts, but with the help of the supervisor.

Literature*:
Compulsory: N/A
Suggested:
Textbook or manual related to the selected programming language or environment.
Textbooks related to the chemical problem.

Title of the course: Practice in computational methods for electronic structure

Credits: 0+2

Coordinator/Department: Prof. Péter Szalay, Physical Chemistry

Terms for joining: Computational methods for electronic structure (lecture)

Topics covered by the course:
This course is a supplement to the lecture "Computational methods for electronic structure" and gives the possibility to use the discussed methods in practice. Different molecular properties will be calculated by several program packages therefore the students will acquire advanced skills in application of electronic structure methods.

Literature*:
Compulsory: Notes on internet in progress
Manuals of the program packages
Suggested:
Attila Szabo és Neil S. Oslund: Modern Quantum Chemistry, Dover Publications, 1996

Title of the course: Quantum mechanics of molecular rotations

Credits: 2

Coordinator/Department: Attila Császár / Physical chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
Angular momentum algebra; group theory of rotations; Euler-angles and direction cosines; coupling of angular momenta; Clebsch-Gordan coefficients; rotational matrices; Wigner-matrices; energy levels and wave functions of rigid rotators; selection rules; deviations from the rigid rotor model; ab initio rotational spectroscopy.

Literature*:
Compulsory:
(1) Császár Attila: Lecture notes (xerox copy, library of ELTE TTK KI).

Suggested:
(1) Harry W. Kroto: *Molecular Rotation Spectra*, Wiley: London, 1975.
(2) Richard N. Zare: *Angular Momentum: Understanding Spatial Aspects in Chemistry and Physics*, Wiley-Interscience: New York, 1988.
(3) P. R. Bunker and P. Jensen, *Molecular Symmetry and Spectroscopy*, 2nd edition, NRC Research Press: Ottawa, 1998.

Title of the course: Quantum mechanics of molecular vibrations

Credits: 2

Coordinator/Department: Attila Császár / Physical chemistry

Terms for joining: Basic knowledge in theoretical chemistry

Topics covered by the course:
Separation of electronic and nuclear motions. The Born–Oppenheimer and the adiabatic approximations. Separation of vibrational and rotational motions: the Eckart conditions. The 1-D harmonic linear oscillator, its solution with traditional and advanced methods. Matrix elements of harmonic oscillator functions. Anharmonic oscillator in one dimension (perturbation theory). Harmonic vibrational analysis for *N*-atom molecules. Normal vibrations. The GF method. The SQM method. Vibrational perturbation theory. Van Vleck transformation. Energy formulae. Resonances. Variational solution of the rotational-vibrational problem. Coordinate systems. General form of the kinetic energy operatorin different coordinate systems. Potential energy hypersurfaces and their *ab initio* determination. Efficient determination of matrix elements. The DVR technique. Diagonalization methods. Normal and local vibrations. *Ab initio* rotational-vibrational spectroscopy.

Literature*:
Compulsory:
(1) Császár Attila: Lecture notes (xerox copy, library of ELTE TTK KI).

Suggested:
Ira N. Levine: *Molecular Spectroscopy*, Wiley-Interscience: New York, 1975
Ira N. Levine: *Quantum Chemistry*, Wiley-Interscience: New York, 1999.

Title of the course: Reaction-diffusion system and its simulation

Credits: 2 + 0

Coordinator/Department: István Lagzi, Physical chemistry

Terms for joining: Basic knowledge in physical chemistry and mathematics

Topics covered by the course:
Chemical reaction, ordinary differential equation and its solution (analytical and numerical solutions). Phases plot, stationary point, linear stability analysis. Diffusion equations, advection equations, partial differential equations, initial and boundary conditions. Analytical and numerical solution methods of partial differential equations. 'Method of lines'; spatial disretization, temporal integration. Finite Element Method (FEM). Chemical patterns. BZ waves,
autocatalytic chemical fronts, FDO, Turing, and Liesegang patterns. Stochastic models, transition probability, Monte-Carlo simulation. Complex systems: reaction-diffusion-advection systems, and theirs modeling, application: air quality models.

Literature*:
Compulsory: Notes on internet in progress
Suggested:
1. Scott, S. K. Oscillations, Waves and Chaos in Chemical Kinetics, Oxford University Press, Oxford, (1995).
2. Epstein, I. R.; Pojman, J. A. An Introduction to Nonlinear Chemical Dynamics, Oxford University Press, New York, (1998).

Title of the course: Responsive nanostructures

Credits:2

Coordinator/Department: Varga, Imre, assistant professor

Deptartment of Physical Chemistry

Terms for joining: beginning terms of the Chemistry Msc., basic knowledge in physical or colloid chemistry

Topics covered by the course:
The course is a lecture covering the following topics: Characteristic features and classes of responsive materials; Bulk and interfacial synthesis of responsive materials. The physical chemistry of responsive materials: thermodynamic and molecular interaction models; The effect of size (from the centimeter to the nanometer range) on the features of the responsive systems; Biocompatible responsive materials; Fields of applications.

Literature:
Compulsory:
Lecture slides and notes. Available in an electronic form on the web site of the course.

Suggested:
Selected English language reviews and papers. Available on the internet.

Title of the course: Second Quantized Formalism

Credits: 2 + 0

Coordinator/Department: Péter Surján, Physical chemistry

Terms for joining: Basic knowledge in physical and theoretical chemistry

Topics covered by the course:
Modern many-electron theory: vacuum state, creation and annihilation of electrons, algebraic formulation of Pauli Principle. Particle number operators. Evaluation of matrix elements. Density matrices. Applications: perturbation theory of electron correlation, intermolecular interactions. The theory of the chemical bond.

Literature*:
Compulsory: Notes on internet in progress
Suggested: P. R. Surján: Second Quantized Approach to Quantum Chemistry, Springer, Heidelberg, 1989

Title of the course: Self-assocation of surfactants in solution

Credits: 2

Coordinator/Department: Gilányi Tibor, Physical chemistry

Terms for joining: Basic knowledge in colloid and surface chemistry

Topics covered by the course:
Physical chemistry of surfactants. The hydrophobic interaction. Driving force of surfactant association..
The theories of micelle formation. Mass action and pseudo phase-separation model. Small systems thermodinamics of micelle formation.
Ionic micellar systems. Problem of the counter-ion dissociation of ionic micelles.
Modification of the mass action model. Distribution of the ions in macroionic systems.
Surfactant aggregation in multicomponent systems. Mixed micelle formation. Solubilizatrion.
Polymer-surfactant interaction. Thermodynamic models. Interaction of surfactants with polyelectrolytes.
Experimental methods. Susfactant activity measurements with ion-selective electrodes. Trace-probe electrolyte method. Static and dynamic light scattering measurements.

Literature*:
Suggested
R. J. Hunter: Foundation of Colloid Science, Clarendron Press, Oxford, 1993

Title of the course: Seminar in Quantum Chemistry - A

Credits: 0+2

Coordinator/Department: Péter Surján, Physical chemistry

Terms for joining: Quantum Mechanics, Theoretical Chemistry

Topics covered by the course:
The students read classical papers of quantum chemistry (in English), and discuss them under the guidance of the seminar leader.

Literature*:
Compulsory: selected papers

Title of the course: Seminar of quantum chemistry B

Credits: 0+2

Coordinator/Department: Prof. Péter Szalay, Physical Chemistry

Terms for joining: Quantum mechanics, Theoretical chemistry

Topics covered by the course:
During this traditional seminar the student reads classical research papers in original (mostly English) language, present them in the front of the class and participate in discussions lead by the professor.

Literature*:
Compulsory: Supporting material provided on the seminars

Suggested:

Title of the course: Special topics in theoretical chemistry

Credits: 2

Coordinator/Department: Attila Császár / Physical chemistry

Terms for joining: Basic knowledge in theoretical chemistry

Topics covered by the course:
Connection between quantum mechanics and classical mechanics: uncertainty relations for macroscopical motions; wave packets as superpositions of wave functions. Time-dependent operators: the Ehrenfest theorem; the virial theorem. Electronic structure of atoms: connection between configuration and state; exact characterization of states; spin-orbit coupling. The Hartree–Fock method: the energy of the H_2 molecule with determinant wave function; the most important steps in the derivation of the HF method. HF methods. Bases in quantum chemical computations: Slater- and Gauss-functions; basis contraction; notation of bases. Accuracy of the Hartree–Fock method (based on data in tables). Electronic structure of transition metal complexes. Crystal-field and ligandum-field theories. Electronic structure of octahedral and tetrahedral complexes. The virial theorem and its spectroscopic consequences. Commutator algebra. Determination of selection rules for simple model systems (potential box, harmonic linear oscillator). Separation of nuclear motion. Lagrange and Hamilton functions and their use in theoretical chemistry. Determination of electronic spectra within the Hückel approximation. Quantum mechnical treatment of spin-spin coupling.

Literature*:
Compulsory:
(1) Császár Attila: Lecture notes (xerox copy, library of ELTE TTK KI).

Suggested:
Ira N. Levine: *Molecular Spectroscopy*, Wiley-Interscience: New York, 1975
Ira N. Levine: *Quantum Chemistry*, Wiley-Interscience: New York, 1999.

Title of the course: Statistical Mechanics 2

Credits: 2+0

Coordinator/Department: András Baranyai, Physical chemistry

Terms for joining: Statistical Mechanics 1

Topics covered by the course:
Optional chapters from statistical mechanics beyond the basics (Liquid theories, transport processes, surfaces, electrolytes, rheology, advanced simulation technologies, etc.)

Literature*:
Compulsory: Lecture notes
Suggested: Baranyai A, Schiller Róbert, Statisztikus mechanika vegyészeknek ,Akadémiai, 2003.

Title of the course: Studies in Material Structure Theory

Credits: 2 + 0

Coordinator/Department: Péter Surján, Physical chemistry

Terms for joining: Quantum Mechanics, Theoretical Chemistry

Topics covered by the course:
Theoretical models and computational techniques in material structure research. Basic physical laws and phenomena (Jahn-Teller theorem, Peierls theorem, etc.). Interpretation of measurements and phenomena. Phenomenology of polymers, crystals, amorphous materials. Geometry and electronic structure. Examples for important families: conjugated polymers, fullerenes, nanotubes, etc.

Literature*:
Compulsory: Notes on internet in progress

Title of the course: The chemistry and physics of flames

Credits: 2 + 0

Coordinator/Department: Tamás Turányi, Physical chemistry

Terms for joining: Basic knowledge in physical chemistry

Topics covered by the course:
Basic notions of combustion science: laminar and turbulent flames, premixed and non-premixed flames, laminar burning velocity; experimental setups for the investigation of flames; chemistry of important combustion reactions: combustion of hydrogen, wet CO and methane, formation of soot in flames, low-temperature hydrocarbon oxidation; generation of nitrogen oxides in flames, methods for the decrease of NO concentration; experimental investigation of the kinetics of gas phase reactions, the features and accuracy of gas kinetic data; simulation of reacting flows: numerical and analytical solution of the balance equations.

Literature*:
Compulsory: PowerPoint files on the Internet
Suggested:

J. Warnatz, U. Maas, R.W. Dibble: Combustion: Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation, Springer, Berlin, 1996

I. Glassman: Combustion, 2nd edition, Academic, Orlando, 1987
S.R. Turns: An introduction to combustion. Concepts and applications, Second edition, McGraw-Hill, Boston, 2000
M.J. Pilling – P.W. Seakins: Reaction kinetics, Oxford Univ. Press, 1995

Title of the course: The Monte Carlo simulation method and its interfacial applications

Credits: 2 + 0

Coordinator/Department: Pál Jedlovszky

Terms for joining: Basic knowledge in physical, theoretical, and colloid chemistry

Topics covered by the course:
The basic background of the Monte Carlo method; Boltzmann-distribution; Metropolis sampling; Monte Carlo simulation on the isothermal-isobaric and grand canonical ensembles; simulation of phase equilibrium: the Gibbs Ensemble Monte Carlo method; potential functions and pair correlation functions; problems of simulating molecular systems; accounting explicitly for the molecular polarizability in the simulation; biased Monte Carlo simulations; Monte Carlo simulations governed by experimental data: the Reverse Monte Carlo (RMC) method; free energy calculation with Monte Carlo methods

Literature*:
Compulsory:
Notes made on the lectures and notes placed to the internet
Suggested:
M. P. Allen, D. J. Tildesley, Computer simulation of liquids
D. Frenkel, B. Smit, Understanding molecular simulations
A. Leach, Molecular modelling

Title of the cours: The XPS technique and its application

Credits: 2

Coordinator/Department: Kiss, Éva, associate professor Department of Physical Chemistry

Terms for joining: beginning terms of the Chemistry MSc., basic knowledge in colloid and surface chemistry (for those having an ELTE chemistry Bsc.: Basics of Colloid and Surface Chemistry, KA2KL1 and KA2KL2; for others: equivalent knowledge)

Topics covered by the course:

Surface analysis in general. The X-ray photoelectron spectroscopy as a surface analytical technique. Principle of the measurement, main parts of the instrument.
Determination of the atomic composition and chemical structure of the surface layer.
Qualitative and quantitative analysis, depth density profile by destructive and nondestructive methods.
Applications in various fields: inorganic, organic systems, determination of the surface coverage and layer thickness using different models.
Additional laboratory practice: demonstration and participation in spectrum analysis.

Literature*:
Compulsory:
B.W. Rossiter, R.C. Baetzold (Eds.) Physical Methods of Chemistry, vol IXB Investigations of surfaces and Interfaces, Wiley, N. Y. 1993.
Bertóti Imre: A felületvizsgálat korszerű módszerei. p.120.
Műszaki felülettudomány és orvosbiológiai alkalmazásai. (Szerk: Bertóti Imre, Marosi György, Tóth András) B+V Kiadó, Budapest, 2003. pp 260-277

Suggested:
W.M. Riggs, J. M. Parker in Methods of Surface Analysis (Ed.: A. W. Czanderna), Elsevier, Amsterdam, 1989. pp. 103-158.

Title of the course: Theoretical basis of physical chemistry laboratory experiments: optical, electrical, magnetic and electrochemical properties

Credits: 2

Coordinator/Department: Győző G. Láng, professor , Institute of Chemistry, Department of Physical Chemistry

Terms for joining: Basic knowledge in mathematics, physics and physical chemistry. Prerequisites are Physical chemistry laboratory (2) or its equivalent, and Advanced physical chemistry laboratory*.

Topics covered by the course:
This course is intended to acquaint the students with the theoretical background of experiments and measuring methods. Considerable effort has gone into linking the content of the course with the topics of “Advanced physical chemistry laboratory”. The goal of the course, is to give a comprehensive picture of this area of scientific activity.
Course Description: Methods based on the interaction of light and material. Advanced spectrophotometry. Methods for the determination of the refractive index. Basic principles of interferometric methods. Polarized light, polarimetry. Complex electrochemical measurements. AC techniques, impedance spectroscopy, evaluation of impedance data. The quartz crystal nanobalance. Determination of dielectric and magnetic properties. Analysis of transient signals and noise. Scanning microscopies, scanning tunneling microscopy.

Literature*:
Wayne R.P.: Chemical Instrumentation, Oxford 1995.
Bard A.J.: Instrumental Methods in Electrochemistry, New York (2001);
Macdonald R.J.: Impedance Spectroscopy, New York (1987);
Böttcher C.J.F.: Theory of Electric Polarization, Amsterdam (1973);

Title of the course: Theoretical tools for molecular spectra and photochemical reactions

Credits: 2+ 0

Coordinator/Department: Prof. Péter Szalay, Physical Chemistry

Terms for joining: Electronic structures of molecules

Topics covered by the course:
This course overviews the theoretical methods which can be used to study the nuclear motion in molecules. In particular, those methods are discussed which can be used to describe molecular spectra and photochemical reactions.

Literature*:
Compulsory: Notes on internet in progress
Reinhard Schinke: Photodissociation Dynamics, Cambridge University Press, 1993
Suggested:

Title of the course: Theory and experimental methods of NMR spectroscopy

Credits: 2

Coordinator/Department: János Rohonczy / Department of Inorganic Chemistry

Terms for joining: entry criteria of MSc. in chemistry

Topics covered by the course:
Topics: Interpretation of NMR phenomenon by vector model and quantum mechanical models in Hilbert- and Liouville-space as well as by product operators. Data acquisition methods: quadrature detection, digital filters. Data processing: Fourier-, Hilbert- and Laplace-transformation, linear prediction. Polarization transfer experiments, adiabatic pulses. Theoretical models of dynamic NMR and NOE phenomena. Modern 2D NMR experiments: inverse detection, phase- and gradient selection. Selective pulse experiments. Diffusion NMR.

Literature*:
Compulsory:
INTERNET: http://vegyszer.chem.elte.hu/nmredu/index.html

Suggested:
P.J. Hore: Nuclear Magnetic Resonance, Oxford University Press, 1995. (ISBN13: 9780198556824, ISBN10: 0198556829)
Atta-ur-Rahman: One and Two Dimansional NMR Spectroscopy, Elsevier, 1989.
S. Berger, S. Braun: 200 and More NMR Experiments, Wiley-WCH, 2004.

Title of the course: Theory of chemical bond

Credits: 2 + 0

Coordinator/Department: Prof. Péter Szalay, Physical Chemistry

Terms for joining: Core courses of chemistry Bsc in theoretical chemistry

Topics covered by the course:
This course provides the qualitative concept which can be used to interpret the chemical bond on the ground of quantum mechanics.

Literature*:
Compulsory: Notes on internet in progress

Suggested:

Optional science course module

Title of the course: Advanced UNIX

Credit: 0+2

Coordinator /Department: Ödön Farkas, associate professor, Department of Organic Chemistry

Lecturer(s): Ödön Farkas, Imre Jákli

Terms for joining: basic informatics skills, user level knowledge of the basic UNIX commands

Topics covered by the course:

How to use the tools of the UNIX operating system, to efficiently solve chemical problems. UNIX shells and graphical environments, workspace customization and setup for special applications, shell programming, regular expressions, AWK programming language. Compilation and installation of programs in UNIX environment.

Compulsory literature: -
Lecture notes

Suggested literature:
Arnold Robbins: Unix in a Nutshell (O'Reilly)

Title of the course: Applied statistics

Credits: 2
Coordinator: Keszei, Ernő

Department: Physical Chemistry

Prerequisits: B.Sc. calculus courses

Topics of the course:

Outline of probability theory basics: Random experiment, random variables. Postulates of probability theory. Expected values and their properties. Stochastic convergence. The law of large numbers. Probability distributions: binomial and Poisson distribution. Identical, exponential and normal distribution. The Poisson process. Chi-squared, Student and Fisher distributions.

Statistics and its application: Population and sample. Sampling methods. Sample statistics. Statistical analysis. Expectation values of populations compared to sample statistics. Estimation methods: maximum likelihood, least squares, moments. Properties of estimators. Confidence intervals. Hypothesis testing: for one expectation, comparing two expectations. More expectations: methods of ANOVA. Comparing variances. Testing isoscedasticity. Statistical models. Linear and nonlinear parameter estimation. Goodness-of-fit tests. Implicit regression. Non-parametric estimation. Outlook to multivariate analysis.

Textbooks to use

Compulsory: J.R.Green, D.Margerison: Statistical Treatment of Experimental Data, Elsevier, 1978

Recommended: William Feller: An Introduction to Probability Theory and its Application, John Wiley, 1971
W. H. Press et al.: Numerical Recipes, The Art of Scientific Computing, Cambridge University Press, 1986
C.Chatfield, A. J. Collins:Introduction to Multivariate Analysis, Chapman and Hall, 1980
Reimann-Tóth: Valószínűségszámítás és matematikai statisztika, Tankönyvkiadó, 1989 (in Hungarian)

Title of the course: Communication in chemistry

Credits: 2

Coordinator/Department: János Tóth, Technical University of Budapest, Physical chemistry

Terms for joining: Basic knowledge of BSc level in computer science

Topics covered by the course:
How to treat technical literature? Which are the most effective methods of verbal and written communication? Lectures will be given and practical exercises provided on the topics. Research tools will also be examined.
What is science? How does the scientific communication proceed? How is the good researcher characterized? What to select as research goal? Design and evaluation of experiments. Ethical questions. Collecting relevant papers in the library, on the net. Publication in science. Formal and informal communication. Conferences, proposals, funds.

Literature*:
Compulsory: Notes on internet (always) in progress
Suggested: Csermely, P., Gergely, P., Koltay T., Tóth J.: Kutatás és közlés a természettudományokban, Osiris, 1999.
Beck M. könyvei.
Dévényi T.: Dr. Ezésez Géza karrierje, Gondolat, Budapest, 1975.
Gyurgyák J.: Szerkesztők és szerzők kézikönyve, Osiris, Budapest, 1996 és később.
Kuhn, Th. S.: A tudományos forradalmak szerkezete, Gondolat, Budapest, 1984.

Title of the course: C programming

Credits: 0 + 2

Coordinator/Department: István Lagzi, Physical chemistry

Terms for joining: ---

Topics covered by the course:

History of C programming. C code structure. Variables and variable manipulations. Command line. Compilation and linking of source code; execution, make, Makefile. Constants, variables and arrays. Operators. Functions. File I/O and binary file I/O. Structures and unions. Pointers. Dynamic allocation of memory, multi-dimensional arrays. Strings, character and bit manipulation. Libraries, functions, global and local variables. Data storage. Mathematical functions. Communication with OS.

Literature*:
Compulsory: Notes on internet in progress
Suggested:
1. B.W. Kernighen, D.M. Ritchie, The C Programming Language, Prentice Hall: 1998

Title of the course: Chemical applications of Fortran C programming languages

Credits: 0+ 2

Coordinator/Department: Prof. Péter Szalay, Physical Chemistry

Terms for joining: Basic course of informatics

Topics covered by the course:
This course provides the basic knowledge of syntax of Fortran and C programming languages, writing, debugging, compiling and running simple codes.

Literature*:
Compulsory:
M. Metcalf és John Reid: FORTRAN 91/95 explained, Oxford University Press, 2000.
Brian W. Kernighan és Dennis M. Ritchie: The C Programming Language, Prentice Hall 1988.
Suggested:

Title of the course: Chemical Data Processing by Java Programs

Credits: 2

Coordinator/Department: Dr. János Rohonczy / Department of Inorganic Chemistry

Terms for joining: entry criteria of MSc. in chemistry

Topics covered by the course:
The aim of this course is an introduction to the modern, object oriented programming language Java. Several examples are used to illustrate the application ability of Java in the chemical research and education: for example, graphic modeling of NMR experiments in WEB browsers, Monte Carlo process simulations on multiprocessor systems, data acquisition and INTERNET based telemetry of laboratory equipments by Java programs.

Literature*:
Compulsory:

http://vegyszer/szervetlen/rj-java/index.html

Suggested:

Nyékiné G. Judit szerk.: Java 1.3 útikalauz programozóknak, ELTE TTK Hallgatói Alapítvány, Budapest, 2001.
D. Flanagan: Java in a Nutshell, 5th Edition O'Reilly & Associates Inc., 2005.
Csizmazia Balázs: Hálózati alkalmazások készítése, Kalibán Kiadó, Budapest, 1999.

Title of the course: Chemical Manager

Credit: 2

Coordinator /Department: István T. Horváth, Professor, Department of Organic Chemistry

Terms for joining: requirements of the Chemistry MSc.

Topics covered by the course:

Introduction to the fundamentals of R&D management
Corporate Strategy
R, D & E Framework
Core Competencies, Competitor Assessment
Strategic Alliances
Technology Strategy Development
Development Strategies

Compulsory literature*:

Chikán Attila: Vállalatgazdaságtan, AULA Kiadó, Budapest, 2000

Internet: www.cordis.lu – Research & Development

Suggested literature:

National Research Council: Linking Science and Technology to Society's Environmental Goals, National Academic Press, Washington D.C.,1996

Title of the course: Chemical Mathematics

Credits: 4 + 2

Coordinator/Department: Péter Surján, Physical chemistry

Terms for joining: Basic Math BSC course(s)

Topics covered by the course:
Chemical application of matrices and vectorial analysis. Multi-dimensional integrals. Differential equations. Function series, Fourier expansion, Fourier transformation. Convolution, Laplace transformation, Orthogonal polynomials. Symmetry operators, group theory.

Literature*:
Compulsory: Notes
Suggested: Bronstein-Semendajev, Mathematical Handbook
Korn-Korn, Mathematical Handbook for Scientists and Engineers

Title of the course: Chemist's Eye-view of Probability

Credits: 2

Coordinator: Nagy, Sándor

Department: Department of Analytical Chemistry

Prerequisites: admission to Chemistry MSc or, alternatively, core mathematics of any BSc program in science or technology

Topics covered by the course:
Distributions of random variables, characterization of distributions, estimation of characteristic parameters, measures of the 'association' of two distributions, sums and products of variables, convolution–deconvolution, random sums, central limit theorem, error propagation, special distributions (Bernoulli, binomial, Poisson, exponential, gamma, normal, χ^2, Cauchy), renewal processes (Poisson process), weighted least squares as maximum likelihood method (example: fitting nuclear spectra).

Literature:
Compulsory:
Nagy Sándor: Nukleáris mérések statisztikája (Valószínűség-számítási összefoglaló alkalmazásokkal). The pdf version of this electronic textbook can be loaded from the website *http://www.chem.elte.hu/Sandor.Nagy/okt/nms/index.html* together with some other documents related to this topic.
Suggested:
Vetier András: Szemléletes mérték- és valószínűségelmélet, Tankönyvkiadó Vállalat, Budapest, 1991
Reimann József: Valószínűségelmélet és matematikai statisztika mérnököknek, Tankönyvkiadó, Budapest, 1992
In English:
Sándor Nagy: Statistical Aspects of Nuclear Measurements. In A. Vértes, S. Nagy, Z. Klencsár: Handbook of Nuclear Chemistry, Kluwer Academic Publishers, Dodrecht, 2003 (Vol. 1, Chapter 7, pp. 325-390.) A legal copy of the chapter can be borrowed from the Coordinator for the semester by those who signed up for the course.

Title of the course: Foundations of modern biology

Credit: 2

Coordinator /Department: Zoltán Gáspári / Department of Organic Chemistry

Terms for joining: -

Topics covered by the course:
Students will get familiarized with the paradigms and current problems of modern biology. They also get a brief overview of several fundamental methods and also of the molecular basis of life. The most widely used biological databases will be introduced as well.

Compulsory literature:
The companion material accessible via WWW.

Suggested literature :
Bálint Miklós: Molekuláris biológia I-II-III.,
Berg-Tymocko-Stryer: Biochemistry, 5th edition
Ernst Mayr: What evolution is

Title of the course: Introduction to Cell biology

Credit: 2

Coordinator /Department: Gábor Réz, ELTE Dept. Anatomy, Cell and Develop. Biol.

Terms for joining: Basics in Chemistry

Topics covered by the course: Prokayotes and Eukaryotes (plant and animal cells), cell nucleus, chromosomes, genes, gene expression, plasmamembrane, receptors, pumps, internal membranes, ribosomes, vesicular transport, endocytosis, intracellular degradation, plant cell vacuoles, receptors, cytoskeleton and cell motility, semiautonomous organelles, cell adhesion, extracellular matrix and plant cell wall, cell cycle, division and differentiation, cell death

Compulsory literature*:
Kovács János: Sejtbiológia, Eötvös Kiadó 1999
Suggested literature:
Szabó Gábor (szerk.): Sejtbiológia, Medicina, 2004
Cooper G. F.The Cell. Sinauer Associates, 2000
Alberts B and oth. Molecular Biology of the Cell. Garland Sciences, 2002
Lodish H and oth. Molecular Cell Biology.Freeman&Co 2000

Title of the course: Particle Physics for Chemists

Credits: 2

Coordinator: Süvegh, Károly

Department: Department of Analytical Chemistry

Prerequisites: basic knowledge in nuclear physics/nuclear chemistry and quantum mechanics

Topics covered by the course:
conservation laws, symmetries, basic forces, properties of force fields, quasi-particles, instruments of particle physics, data bases, virtual particles, bosons, Feynmann graphs, quarks and particles, colors of particles, particles and the Universe

Literature*:
Suggested books:
Harald Fritzsch: Quarks, *Penguin Books*, London, 1992
http://particleadventure.org/index.html
Martinus J G Veltman: Facts and Mysteries in Elementary Particle Physics, World Scientific, London, 2004

Title of the course: Physics (2)

Credits: 2+0

Coordinator/Department: Jenő Kürti, Biological Physics

Terms for joining: Physics (1) BSC course

Topics covered by the course:

Electrostatics in vacuum
Magnetostatics in vacuum
Electric– and magnetic multipoles
The motion of charged particles in electric– and magnetic fields
Electric– and magnetic field in materials
Time dependent electric– and magnetic fields
Maxwell's equations
DC and AC phenomena
Electric transport properties of materials
Energy of the electromagnetic field
The light – elecromagnetic waves

Literature *:
Compulsory: Notes on internet, partly available, partly in progress
Suggested:
– Basics of Physics, Eds. Erostyák János and Litz József, Tankönyvkiadó, Budapest
– Physics II, Ed. Litz József, Nemzeti Tankönyvkiadó, Budapest 2005
– The Feynman Lectures on Physics, R.P. Feynman, R.B. Leighton, M. Sands, Műszaki Könyvkiadó, Bp.1970

Title of the course: Quantum Mechanics

Credits: 2 + 2

Coordinator/Department: Péter Surján, Physical chemistry

Terms for joining: Chemical Mathematics

Topics covered by the course:
Physical observables as Hermitean operators. Wave functions. Probability interpretation. Schrödinger equation. Perturbation theory. Electron spin, Pauli principle. Electronic structure of atoms. Scattering theory. Simple molecules; formation of chemical bonds.

Literature*:
Compulsory: G. Marx: Kvantummechanika (in Hungarian), or: any standard textbook in English

Title of the course: Quantum Mechanics: Theoretical Problems, Problematic Theories

Credits: 2

Coordinator: Süvegh, Károly

Department: Department of Analytical Chemistry

Prerequisites: BSc-level knowledge in quantum mechanics

Topics covered by the course:
axioms of quantum mechanics, immediate consequences, interpretations of reality, EPR-paradox, quantum teleportation, quantum cryptography, hidden variables, Bell-theorem, Bohm's quantum potential, measurement theory, energy-time uncertainty, natural linewidth, “classic” spin, Dirac's equation, relativistic spin

Literature:
Suggested books:
Ballentine: Quantum Mechanics, *Prentice Hall*, Englewood Cliff, 1990
Wheeler, Zurek: Quantum Theory and Measurement, *Princeton University Press*, Princeton, 1983
D. Bohm: Quantum Theory, *Dover Publications*, 1989

Title of the course: Scientific American – the International Language of Chemistry

Credits: 2

Coordinator: Nagy, Sándor

Department: Department of Analytical Chemistry

Prerequisites: basic command of English

Topics covered by the course:
Students can sign up for the same course several times for 2 credit points each time, because apart from the introductory part that is repeated in each semester (communication by e-mail, writing CVs, etc.) the seminar is based on the active participation of students. They are supposed to write short essays on various topics in chemistry, do translation to and from English and give oral presentations.

Literature:
Compulsory:
None.
Suggested:
John Daintith: A Dictionary of Chemistry, Oxford University Press, New York, 2004
Peter William Atkins and J. A. Beran: General Chemistry, Second Edition, Scientific American Books, N. Y., 1992
D.D. Ebbing, M.S. Wrighton: General Chemistry, Houghton, Dallas, 1987
Selected Classic Papers from the History of Chemistry (http://web.lemoyne.edu/~GIUNTA/papers.html)
Chemistry, the Central Science 7/e by Brown, LeMay, and Bursten (http://cwx.prenhall.com/bookbind/pubbooks/blb/)
Student Website for Chemistry: The Science in Context (http://www2.wwnorton.com/college/chemistry/gilbert/home.htm)
αlphαDictionary.com • Free Chemistry Dictionary (http://www.alphadictionary.com/directory/Specialty_Dictionaries/Chemistry/)

Title of the course: Scripting

Credits: 2

Coordinator/Department: Gabor Magyarfalvi, Department of Inorganic Chemistry

Terms for joining:

Topics covered by the course: Advantages and applicability of very high level programming languages (scripting) to scientific problems. This is a course intended for laymen, not future programmers. The objectives are to provide practical help enabling them quickly and flexibly process all kinds of data, automate their interaction with computers. Instruction is through application examples from chemical research.
The fundamentals of two programming languages, Python and Perl, often used programming constructs, text processing, numerical and user interface libraries are covered.

Literature*:
Compulsory:

Suggested:
- H. P. Langtangen: Scripting for Computational Science, Springer, 2004
- M. Pilgrim: Dive into Python, Apress, 2004
- D. M. Beazley: Python Essential Reference, New Riders, 2001
- L. Wall, T. Christiansen, R. L. Schwartz: Programming Perl, O'Reilly , 1996

Title of the course: Supplementary chapters in Physics I. (classical mechanics – quantum mechanics)

Credits: 2 + 0

Coordinator/Department: Jenő Kürti, Biological Physics

Terms for joining: Physics (1), Physics (2) BSC courses

Topics covered by the course:
Basic experiments to quantum physics
Lagrange- and Hamiltonian-formalism in classical- and quantum physics
Bohr-Sommerfeld quantization in phase space
de Broglie's matter waves
Wave mechanics (Schrödinger) – matrix mechanics (Heisenberg)
Poisson-bracket – commutator
Commutation relations, uncertainty relations
Symmetries and physical quantities
Two-slit interference
Harmonic oscillator in quantum mechanics
Angular momentum in quantum mechanics

Literature*:
Compulsory: Notes on internet, partly available, partly in progress
Suggested:
– Erostyák János, Kürti Jenő, Raics Péter, Sükösd Csaba: Physics III, Nemzeti Tankönyvkiadó, 2006 (Chapter VI.: Atomic Physics)
– R.P. Feynman: The Feynman Lectures on Physics, volume 3. (chapters 26., 37. and 38.), volume 6. (chapter 71.), Műszaki Könyvkiadó, 1969
– Marx György: Quantum Mechanics, Műszaki Könyvkiadó, 1971

Title of the course: Supplementary chapters in Physics II. (Relativity)

Credits: 2 + 0

Coordinator/Department: Jenő Kürti, Biological Physics

Terms for joining: Physics (1), Physics (2) BSC courses, Supplementary chapters in Physics I MSC course

Topics covered by the course:
Classical electrodinamics
History of relativity
Invariant and covariant description of spacetime
Relativistic kinematics – the Lorentz-transformation
Relativistic dinamics – matter vector (energy-momentum vector)
Vectors and tensors in space-time
Relativistic electrodynamics
Dirac-equation – the spin
Basic concepts of general relativity

Literature*:
Compulsory: Notes on internet, partly available, partly in progress
Suggested:
– Erostyák János, Kürti Jenő, Raics Péter, Sükösd Csaba: Physics III, Nemzeti Tankönyvkiadó, 2006 (Chapter V.: Relativity)
– R.P. Feynman: The Feynman Lectures on Physics, volume 2. (chapters 15-7.), volume 3. (chapter 34.), volumes 5. and 6. Műszaki Könyvkiadó, 1969
– E.F.Taylor - J.A.Wheeler: Spacetime Physics, Gondolat Kiadó, 1974

Title of the course: The History of Chemistry

Credits: 2

Coordinator/Department: György Inzelt, Department of Physical Chemistry

Terms for joining: knowledge of the basics in the BSc in Chemistry training

Topics covered by the course: The milestones in chemical way of thinking and technologies. The most famous chemists from the ancient times to the end of the 20^{th} century. The development of natural philosophy during centuries. The chemistry in the Bible and Pliny, the elder books. Alchemy and alchemists. The beginning of modern chemistry. Atomistic theories. Elements and their discoveries. Conservation laws. The birth and development of subdisciplines: chemical thermodynamics, electrochemistry, reaction kinetics, aniline and organic dyes and medicines. Chemical symbols. Periodic tables. The advance of chemical methods and technologies. Chemistry and environment. From the vis vitalis to the gentechnologies. The development of scientific communication (universities, journals, conferences)

Literature*:
Compulsory: K.J. Laidler: The World of Physical Chemistry, Oxford Univ Press, Oxford, 1993.
J. Hudson: The History of Chemistry, MacMillan, London, 1992.
Suggested: J.R. Partington: A History of Chemistry I-IV, MacMillan, London, 1964
and original publications of the most famous chemists.