Chemistry, PhD

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Available PhD Programs in the field of Chemistry:

- Reaction Kinetics and Catalysis
  Head of Program: Prof. Ferenc Joó
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- Coordination and Analytical Chemistry
  Head of Program: Prof. István Fábián
  e-mail: ifabian@science.unideb.hu
- Macromolecular and Surface Chemistry
  Head of Program: Prof. Sándor Kéki
  e-mail: keki.sandor@science.unideb.hu
- Chemistry and Chemical Biology of Carbohydrates and Heterocycles
  Head of Program: Prof. László Somsák
  e-mail: somsak.laszlo@science.unideb.hu
- Research on Didactics of Teaching Chemistry
  Coordinator: Dr. Zoltán Tóth
  e-mail: toth.zoltan@science.unideb.hu

Length of the program: 4 semesters

The following items will be considered and scored during the (oral) admission process:

	Hungarian Applicant MSc Diploma	**Hungarian Applicant MSc Diploma 3+ years old or Foreign Applicant**
Proficiency in Chemistry	(max. 40 pts)	(max. 55 pts)
Quality of the Diploma	(max. 30 pts)	not considered
Previous scientific activity (research papers, lectures, posters, etc.)	(max. 30 pts)	(max. 45 pts)

A successful applicant should reach a minimum of 60 points (total).

Reaction Kinetics and Catalysis

This program offers research possibilities in the following areas of interest: *Nonlinear Chemical Dynamics:* Dynamic instabilities (e.g., bistability, oscillations and chaos) in chemical systems; pattern formation in reaction-diffusion systems. *Homogeneous and Heterogeneous Catalysis*: Catalysis by organometallic complexes in aqueous solution; synthesis of new ligands and complexes (e.g. water-soluble complexes with N-heterocyclic ligands); study of hydrogenation, hydration, redox isomerization, hydrogen storage and generation, and similar reactions; heterogenization of soluble catalysts and synthesis of colloidal (nanosized) metal catalysts; catalysis in flow devices; modification of biomembranes by hydrogenation. *Computational Chemistry*: application of high level QM, QM-MM, DFT, etc. methods for establishing molecular structures and possible reaction mechanisms in catalytic processes. *Kinetics and Mechanisms of Photochemical Reactions.*

Coordination Chemistry

The program includes bioinorganic chemistry focusing on the thermodynamic and structural characterization of the transition metal complexes of amino acids, peptides and derivatives. Metal complexes of hydoxamate based ligands are the most promising molecules for the modeling and inhibition of metalloenzymes. Research on new MRI contrast agents is a rapidly growing area in this program. These studies are based on the equilibrium, kinetic and structural investigations of the lanthanide complexes of various macrochelates. Polynuclear complexes containing metal-metal bonds (e.g. Pt-Tl, Pd-Tl, Pt-Sn, etc.) also comprise a significant part of the program. The studies on the organometallic compounds of ruthenium and other platinum metals provide an insight into the structural versatility of these complexes and may contribute to developing new anticancer agents. Another research area covers the kinetics and mechanisms of environmentally relevant redox reactions. The catalytic roles of metal ions and their complexes are of particular significance in many of these systems.

Environmental Instrumental and Analytical Chemistry

In this program, students participate in several courses on instrumental or environmental chemistry and they are involved in research activities on numerous modern topics that are pursued at our institute. The three main research areas are as follows: *i*) elemental and speciation analysis in environmental samples, *ii*) developing electromigration separation techniques in capillary and microfluidic devices and *iii*) bioanalyis with chromatographic methods. These research topics include basic research aspects like studies of thermic decomposition of compounds with a newly developed technique, “thermospectrometry” or designing microfluidic chips applicable for ultrafast separation. The instrumentation includes commercially available sophisticated equipments and locally developed modern devices for the determinations of elements, inorganic ions, pharmaceuticals and proteins in a large variety of environmental and clinical samples.

Macromolecular and Surface Chemistry

Macromolecular Chemistry: Designed polymers are in the focus of today’s technology and material science. Using telechelic polymers special polymer systems like linear or star shaped amphiphilic copolymers and polymer networks can be prepared. Conjugated polymers combine the mechanical properties (flexibility, toughness, malleability, elasticity, etc.) of plastics with high electrical conductivity. Their present and future applications are based on such unique properties as electric conductivity, electroluminescence, molecular magnetism,

photoluminescence and so on. During the program the applicants can master modern polymer synthesis methods such as living cationic/anionic polymerization, ROMP, ATRP as well as Suzuki polycondensation. In our complex material testing laboratory the structure determination of complex and special synthetic and/or natural macromolecules and the mechanical testing of plastics as well as composite structural materials can also be carried out. Based on our advanced mass spectrometric infrastructure structure determination based on fragmentation is conducted. Joint techniques such as HPLC-MS and/or HPLC-MS^2 measurements using *off-line* or *in-line* sample introduction methods enable the investigation of peptides, oligosaccharides, synthetic polymers, low molecular weight (<1000 Da) organic molecules, drugs, side products and metabolites.

Surface chemistry: Research on macromolecular colloids involves preparation and functionalization of poly(amino acid) polymers, their partial hydrophobisation for the modification of the tertiary structure; analysis and characterization of the resulting ligand structure in solution using multinuclear and multidimensional NMR spectroscopy; equilibrium, structure and dynamics of metal complexes with macromolecular ligands in solution. In the research area of interfacial reactions the applicants can study the binding of important micro-elements, contaminating ions and radioactive cations on the surface of clay minerals by radioindication method. One can also study the mechanism of catalytic reactions on clay surface. The goal is the preparation of radiolabeled amino acid derivatives and their stable complexes with radionuclides used in medical diagnostic imaging (^{99m}Tc, ^{111}In, ^{67}Ga, ^{53}Sm, ^{90}Y). The three branches of solution-state NMR spectroscopy are capable of the investigation of solids, sols and gels. Using NMR cryoporosimetry the pore size of both soft and hard porous materials can be determined, provided the pore size is less than 100 nm. Our PhD students are able to investigate the swelling of macromolecular colloids and the pore size of carbon nanoparticles and carbon-based gels with this technique. NMR diffusiometry is an important tool for the analysis of larger pore sizes and pore structures. The applicants can learn through this technique the aspects of structure and adsorption behavior of solids and gels. The low and high-resolution NMR relaxometry is suitable for the investigation of the size and dynamics of colloids. This method enables for the applicants the characterization of carbon nanoparticles, as well as dilute polymer solutions. The involvement of new quadrupole NMR nuclei (^{23}Na, ^{17}O) can further broaden the perspectives.

In the future, the applicants will have the opportunity to learn solid-state NMR as well. All the necessary hardware has already been installed.

Chemistry and Chemical Biology of Carbohydrates and Heterocycles

Heterocycles represent more than half of the known organic compounds and form the basic scaffold of numerous families of natural products e. g. flavonoids, alkaloids, antibiotics. They play fundamental roles in biochemical processes of living organisms. Most natural and synthetic drugs as well as agrochemicals contain at least one heterocycle whose preparation in an efficient and stereoselective manner is a major challenge for synthetic organic chemistry.

Carbohydrates (glycans) – the most widespread compounds with the biggest mass on Earth – may also appear as heterocycles. The study of carbohydrates, due to mutual interactions between several fields of science (e. g. synthesis, analytics, biochemistry, biomedicine, materials science), is being nowadays integrated into a complex approach called glycoscience.

Biological roles of heterocycles and carbohydrates are mostly realized by their interactions with macromolecules e. g. proteins recognizing or/and transforming (small) molecules or inducing immune responses (receptors/lectines, (glyco)enzymes, antibodies, respectively). Study of such interactions in a *chemical biology* approach may yield informations on essential properties of the interacting system to be utilised among others in drug design.

Based on this background the program offers *education and research* in the following main areas: synthesis of carbohydrate containing compounds of natural origin and their core scaffolds; design and synthesis of glycomimetics and enzyme inhibitors; study of mechanisms of action of glycoenzymes; investigation of carbohydrate–protein interactions by up-to-date instrumental methods; synthesis, selective transformations and structural elucidation of potentially pharmacologically active natural O-heterocycles (e. g. flavonoids, chromonoids, coumarins), their sulfur-containing analogues and O,N-heterocycles.

For a more detailed listing and description of the courses and research topics, please, consult http://www.chem.science.unideb.hu/Dprog_K5_en.html

Research on Didactics of Teaching Chemistry
The aim of this program is to studying the role and methods of education in shaping the attitude to and knowledge of chemistry of both the young and adult generations.

For admission enquiries please check http://englishstudies.sci.unideb.hu
or send a message to englishstudies@detek.unideb.hu