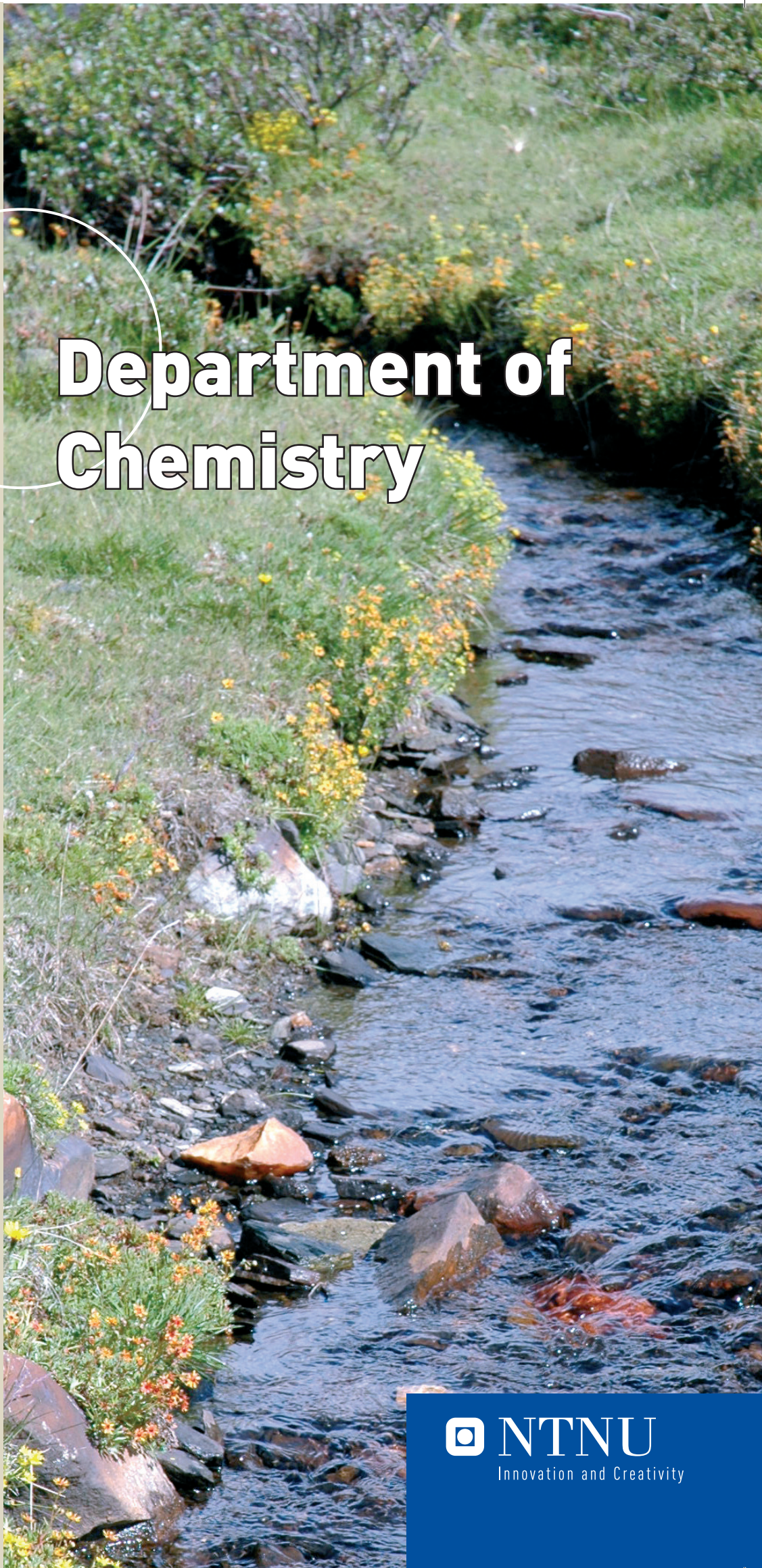


Annual Report 2005

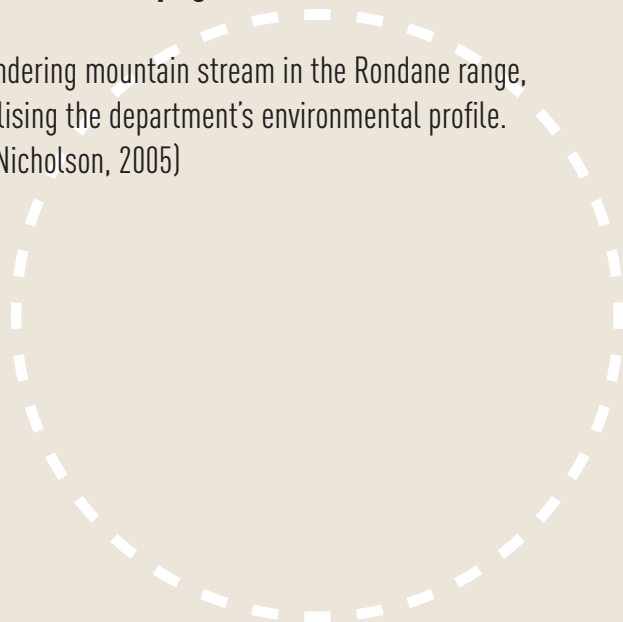
Department of Chemistry



DEPARTMENT OF CHEMISTRY, NTNU

Picture on front page:

A meandering mountain stream in the Rondane range, symbolising the department's environmental profile.
(D. G. Nicholson, 2005)



Annual Report for

Department of Chemistry
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Norwegian University of Science and Technology
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Staff photos David Nicholson, except:
photo on Derek Chadwick found on his web-site www.novartisfound.org.uk



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Foreword

The Department of Chemistry is proud to be the leading department within NTNU for publishing the most research papers per academic staff member ("Universitetsavisa" 28.02.06), but we cannot rest on our laurels. The Department is more than the sum of its parts, but this is not enough. There has to be a corporate will to work together, to get things done, and do them well.

2005 is the year when NTNU moved into a governance based on the concept of unified leadership with appointed instead of elected Rector and Deans. However, a vestige of the previous democratic system still exists in that the Heads of Departments are elected.

The changeover was implemented in October and is particularly significant for the department because the outgoing head, Professor Knut Schrøder, had occupied the position for thirteen years and given sterling service. It was therefore particularly fitting that this transitional milestone was marked by the department in a ceremony thanking Knut for his efforts on behalf of the department.



Anne Langseth, David Nicholson and Knut Schrøder

The University Board has a vision of NTNU being the highest ranked Norwegian university and amongst the ten best in Europe. This is a very ambitious goal and requires considerably improved funding if it is to be attainable. Is NTNU's goal a realisable vision or an unattainable dream? If the former, then the economic conditions we operate under must change for the better – and quickly. After all, the Board expressly aims for NTNU to be in the company of world renowned universities which receive grants greatly in excess of those received by Norwegian universities. For example, the premier European technical university (Imperial College, London) receives funds that are four times more per student than NTNU and EPFL, Lausanne which is ranked tenth receives three times more.

Nevertheless, the department is focusing as best it can on maintaining and raising quality in research and teaching. This brings up the subject of our strategies with regard to research. The department is in need of an updated Strategic Plan. We need to set out our vision for the future. Therefore, formulating effective strategies will be the focus of the department's seminar to be held at Bårdshaug Hotel in February 2006. A significant part of this seminar will be to define and assess the factors that together define the size of the department.

This is becoming increasingly relevant because the department has a relatively high average age for the academic staff. This means that a stream of staff will be retiring over the next five years or so. This makes it possible for the department to meet changed requirements through strategic restructuring in accordance with the Strategic Plan, a process that began in 2005.

The BSc. programme started in 2003 and there appears to be a trend for increasing numbers of admitted students. On the other hand, the corresponding numbers on the technology (sivil ingeniør) side are static. As for PhD's, the department is satisfied that eight doctorates completed their studies in 2005 and especially since four of them are women.

David Nicholson



Swiss-Norwegian Beamlines at ESRF – 10 Years of Successful Operation

The year 2005 also marked a milestone in the Department's activities within structural chemistry when the Swiss-Norwegian Beamlines (SNBL) at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France celebrated the tenth anniversary of experiments since commissioning. Actually, the Department's engagement in SNBL started as far back as 1990 when Professor Frode Mo of the Department of Physics (then NTH) and Professor David Nicholson of the Department of Chemistry (then AVH) joined forces to start the project with a grant of NOK 2 million from the University of Trondheim as it was then. The University of Lausanne is NTNU's counterpart on the Swiss side. The SNBL consortium is a 50:50 Norwegian:Swiss collaboration and comprises the following partners: NFR, NTNU, the universities of Oslo, Stavanger, Tromsø, Lausanne, Berne, Geneva and ETH, Zurich.

SNBL has a contract with the ESRF as a Collaborative Research Group (CRG). The ESRF itself is an impressive example of European collaboration in science; eighteen nations work together to use the extremely bright beams of light produced by the high-performance storage ring. A remarkable range of materials are studied from biomolecules to nanomagnets, from ancient Egyptian cosmetics to metallic foams.

SNBL is really a research institute with a local staff of seven plus two postdocs. In addition researchers from the participating universities carry out their studies there. SNBL is in effect a home synchrotron laboratory for NTNU. Construction of the beamline

was finished in mid 1994 and the first experiments with beam were carried out in October, '94.

The beamline is split physically into two branches that can be operated independently. SNBL is the most productive of the fourteen CRGs and in full operation produces about 950 eight-hour shifts annually on the two branch lines. Allocation of shifts breaks down into about 630 for SNBL's own users with the remaining 310 shifts being allocated according to the contract by ESRF to general users. The numbers show variations due to periods of upgrade and maintenance and installation of new equipment. The beamtime provided by SNBL to its users constitutes about 2/3 of Norway's total share at the ESRF

The first 10 years of operation have proved the SNBL to be a very profitable investment for many fields of science both in Norway and Switzerland, as for instance solid state physics and chemistry, materials science, biocrystallography, diffraction physics and mineralogy. The two beamline branches have been used for a wide variety of crystallographic and spectroscopic experiments. Currently work is being carried out on upgrading the XAFS facility. This also includes incorporating a Raman spectrometer for carrying out simultaneous measurements with XAFS and XRD. The system will be tested early in 2006.

Information on the Swiss-Norwegian Beamlines is available at the SNBL website:

http://www.esrf.fr/exp_facilities/BM1A/index.htm

David Nicholson



An aerial view of The European Synchrotron Radiation Facility (ESRF), Grenoble France. The storage ring has a circumference of 872 meters. Courtesy of the ESRF.

Ultra-trace element analysis by high resolution ICP-MS

Double focusing magnetic sector field inductively coupled plasma-mass spectrometry (HR-ICP-MS for short, HR for high resolution) is the most powerful analytical technique for multielement analysis at low concentrations. In October 2004, a HR-ICP-MS instrument was installed in a dedicated room in the Department of Chemistry areas in Realfagbygget. The instrument was financed through a grant for advanced scientific equipment (The Research Council of Norway/NTNU), and is jointly owned and operated by the Department of Neuroscience and the Department of Chemistry. The total costs, including some extra equipment and building construction, were 4.3 million NKR.

Most ICP-MS instruments in use today are not of the high resolution type, but are equipped with a single quadrupole mass filter. Commercial instrumentation of this type became available in 1984. The main limitation of quadrupole ICP-MS is limited mass spectral resolution. Thus, determination of several isotopes, in particular those

with mass-to-charge ratios between about 40 and 80, is prone to spectral interferences, especially when analysing heavy matrix materials such as biological samples. In January 1995, the first routine HR-ICP-MS instrument, the Finnigan Element1, was launched on the market. High resolution instruments offer a much better mass resolution than quadrupole instruments, through a two-step separation process (Figure 1): The ion beam passes first through a magnetic sector field which is dispersive for ion mass and energy, then through an electric sector analyzer which is dispersive with respect to ion kinetic energy. In 1998, the follow-up version Element2 was launched, and Thermo Electron Corporation in Bremen is still the sole commercial provider of HR-ICP-MS instruments today. Norway is a high-density area for ICP-MS instruments: Worldwide, a total of 109 Element1 and about 300 Element2 instruments have been sold, 8 (2 Element1 and 6 Element2) are in operation in Norway.

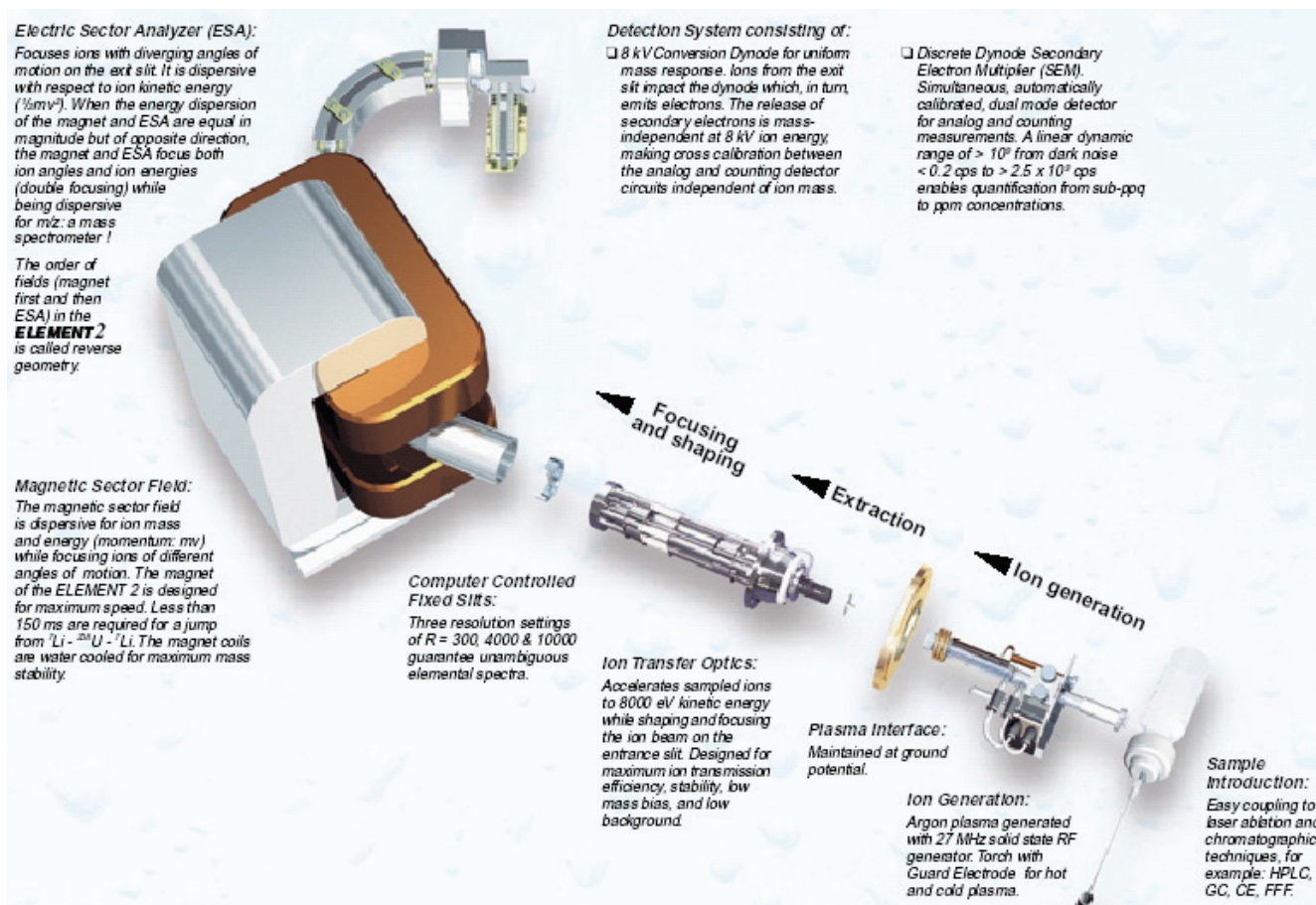


Fig. 1. Principles of operation for the Finnigan Element2 high resolution ICP-MS instrument (Thermo Electron Corporation, Bremen).

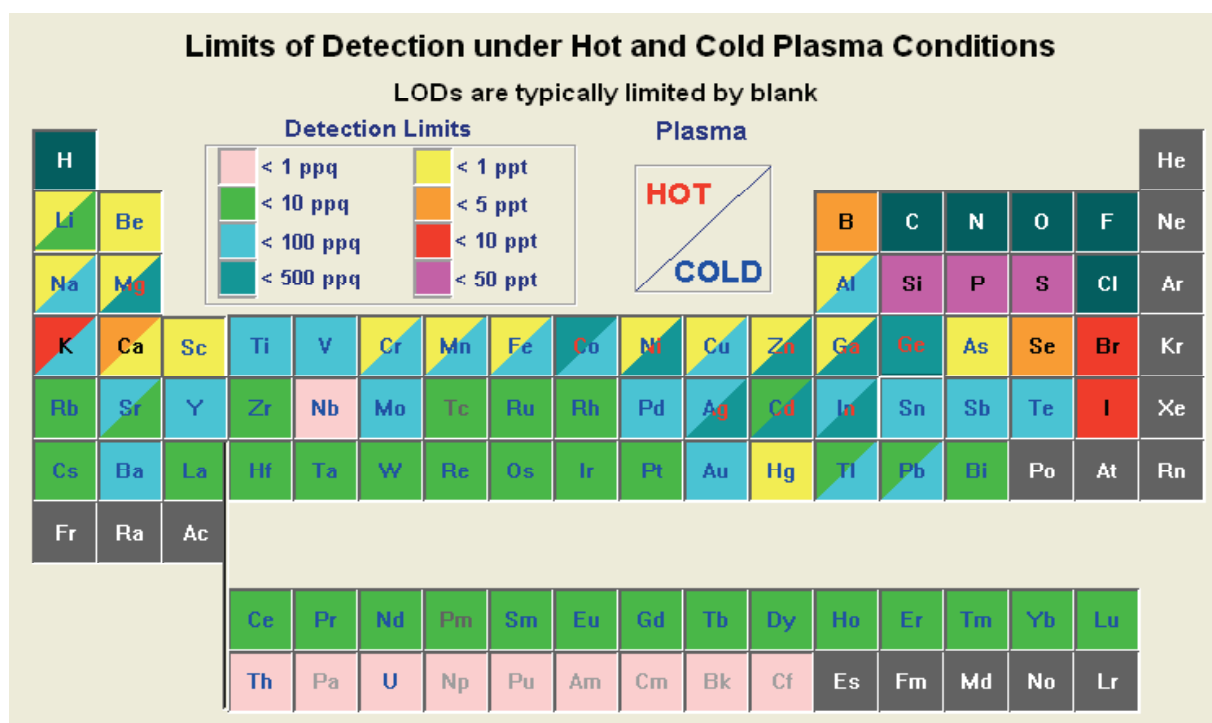


Fig. 2. Elements that can be measured by the Finnigan Element2 high resolution ICP-MS instrument, and respective detection limit ranges (ppt = ng/L, ppq = pg/L) (Thermo Electron Corporation, Bremen).

Practically all types of materials can be analysed, but the samples have to be in solution. Thus, all types of solid samples have to be decomposed before analysis, usually by adding strong acids and heating under pressure in a microwave oven.

The superior mass resolution of the HR-ICP-MS combined with its unrivalled sensitivity enables interference free measurement of almost the whole periodic table and in almost all matrices, covering a mg/L (ppm) to pg/L (ppq) concentration range in one single sample run. Detection limits (Figure 2) below 1 pg/L can be achieved for certain elements. In most cases, the detection limit is not limited by the instrumental background signals, but by the blank levels (amounts of the relevant element in reagents, as contaminant in the laboratory air, etc.).

As an example of the sensitivity of the method, we had no problems quantifying gold in samples from the river Nidelva at about 0.1 ng/L (0.0001 ppb). Thus, Nidelva supplies around 500 g of gold to the Trondheimsfjord each year.

In addition to determination of elemental concentration, the other main application of the instrument is isotope ratio measurements. There are other instruments on the market dedicated to isotope ratio measurements, but these are more expensive, more complex in use, and are not suited for elemental concentration measurements. Thus, as a combination instrument the Element2 is the preferred choice. Some key elements for isotope ratio measurement are Pb, Sr, Pu and Fe. As an example, we analysed some sediment samples from the Kola Peninsula in Russia for the $^{240}\text{Pu}/^{239}\text{Pu}$ ratio. All plutonium in the environment is anthropogenic (man made). The isotope ratio is

slightly different for plutonium originating in nuclear explosions, in nuclear power plants or in fuel reprocessing plants, respectively. The isotope ratios in the Kola samples showed clear geographic variation, demonstrating that the plutonium at different places came from different sources. The analytical precision was adequate to clearly discriminate between the different plutonium sources, even at the low existing concentrations of 1-55 ng/L. Another example is determination of the $^{206}\text{Pb}/^{207}\text{Pb}$ ratio, which was successfully applied to show that almost all Pb in the organic surface layer of natural soils in Norway is of pollution origin, even in areas very far from major pollution sources.

From January 1, 2005 to April 20, 2006, the Department of Chemistry has used the instrument for a total of 500 hours (actual analysis of samples with the plasma burning). The total number of samples analysed are 2486, meaning that the instrument has produced nearly 60,000 analytical figures during this period (an average of 24 elements determined in each sample). 568 of the analysed samples were from external sources (other Departments at NTNU and various external institutions, especially SINTEF), earning the Department a total of about 210,000 NKR.

With this instrument the Department (and also partly other NTNU departments and SINTEF) has entered a new era in multi-trace element analysis. The possibilities and applications are many, and we will make sure that the instrument continually will earn its place both as a workhorse and as a core in new developments in the future.

Syverin Lierhagen and Trond Peder Flaten

Simple, cheap and hopefully understandable

Chemistry as a subject has its history and identity well embedded in the laboratory. It has been said that the chemist thinks with his hands, testifying to the importance of the practical aspects of chemistry as a subject. Chemistry education in schools often suffers from lack of, as well as inadequate, equipment. At the same time investigations show that both teachers and students/pupils value experimental work the most.

Many of the experiments used today are old (that is more than 100 years), with which there is nothing wrong per se. However, quite some experiments also harbour logical and pedagogical flaws. This area of investigation is seldom prioritised, although the impact of improved experiments would be large, as many children and youths would thereby enjoy and comprehend more in their chemistry classes.

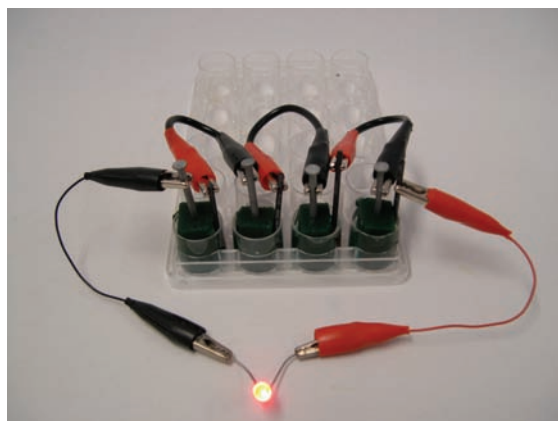


Fig. 1. The battery consists of four cells connected to a light diode. Each cell is made from a pencil rod, a galvanised nail, copper(II)sulphate solution and sodium sulphate solution (absorbed in floral foam).

A collaboration between The School Laboratory of Science and Technology at NTNU (by Per Odd Eggen), the School Laboratory for Chemistry at the University of Oslo (by Truls Grønneberg) and the Department of Chemistry (by Lise Kvittingen) at NTNU has for some years worked on the investigation and development of illustrative experiments for this purpose. The aim is to make more logical and illustrative experiments by using cheap materials and small amounts of chemicals as well as set-ups that comply with the rigour of health and environmental demands of today. The results of his collaboration have resulted in the front cover of *Journal of Chemical Education* showing an apparatus for electrolysing water for the price of less than one euro.

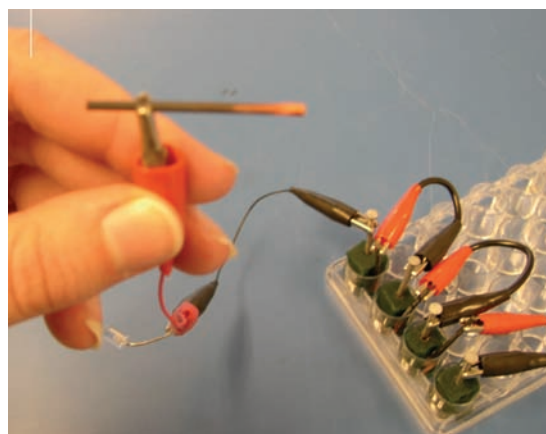


Fig. 2. The figure shows a copper layer deposited onto one of the pencil rods after a short while.

This year two papers on galvanic cells have been accepted by the *Journal of Chemical Education*. The materials needed to make these are some metal wires, nails, pencil leads, floral foam, culture plates, light diodes and some simple solutions- all at a combined cost of less than a euro- and the material can be reused.

Lise Kvittingen

Computerised quality control of protein gels

It is important to know the biological functions of genes in medicine and biology. To obtain this information it is common to inspect how the genes are switched on or off (i.e. expressed) in relation to different biological conditions. A gene is expressed when special proteins read off the DNA sequence of a gene and translate that into mRNA. The mRNA is then transported out of the nucleus to the ribosome where it is used for production of a protein. The proteins are important because they represent the type of molecule which is responsible for most of the biological functions in a cell. Thus it is of great interest to measure the concentrations of the different protein molecules and one of the most commonly used methods are based on

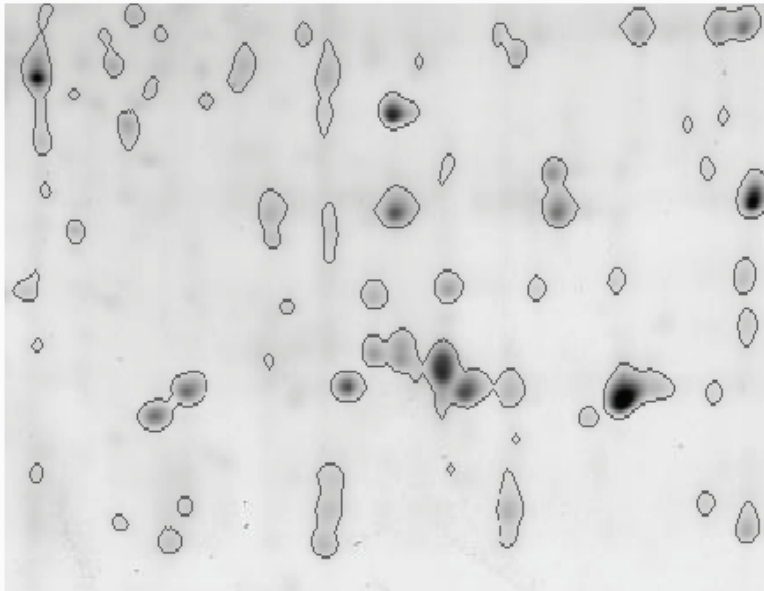


Fig. 1. How segmentation can isolate the pixels within different spots on a protein gel

2-dimensional electrophoresis. This is a technique where a gel-like surface separates the proteins in two dimensions. Along the first dimension the proteins are separated according to their isoelectric points. This corresponds to the pH concentration where a molecule does not contain an electrical charge. A pH gradient is produced along one dimension in an electrical field such that the charged proteins can migrate either to the negative or the positive poles. At the pH value corresponding to their isoelectrical point, the proteins become neutral and will stop their migration. Along the second dimension the proteins are separated according to their masses. To enable visual detection of the protein spots, silver atoms are added which attach themselves to a specific amino acid on the different proteins. The result is a 2 dimensional map of black spots where each spot corresponds to a protein.

When all the proteins in a cell are investigated, thousands of spots on the electrophoresis gel will be shown. When the protein productions under different biological conditions are compared, it is necessary to compare these 2-D maps. Unfortunately, this is hampered by the fact that the gels have been stretched and added various types of artefacts during their use. Humans are able to visually detect likely protein spots and non-protein spots on the gel, but this is a very time consuming and expensive process, especially when a large number of gels need to be compared. Therefore a more fruitful approach is to use computers to perform the analysis.

In this project the PhD student Morten Beck Rye has developed a computer program which is able to reproduce much of the human ability to distinguish true protein spots and non-protein spots. This has been done by teaching a computer program from examples of gels together with the human classifications of the spots. To measure protein and non-protein spots we have concentrated on separating isolated (protein) from overlapping spots (which is usually non-protein). Overlapping spots which also handles overlapping proteins will be studied later. The method is started by performing a segmentation to obtain the pixels corresponding to spot regions on a gel. Then the different spots are classified into isolated or overlapping spots according to the shape of their boundaries. To do this a representation of the boundaries is

required. Here the distances from the centre point of a spot to the boundary pixels at predefined angles is used. In this study each boundary was represented by 200 angle-distances. 14 overlapping and 39 isolated spots described by 200 variables were collected in a data matrix with 53 rows 200 columns. Associated with each row was its class membership (isolated or not) which was coded as 0 or 1. Discriminant partial least squares regression (DPLSR) was used to create a computer model which was able to simulate the ability of a human to discriminate between overlapping and isolated spots.

Such computer models can form a part of a larger system for analyzing large amount of protein gels and spots which hopefully will eliminate the need for manual inspection. Our computer models will therefore make this process much cheaper and faster.

Bjørn K. Alsberg

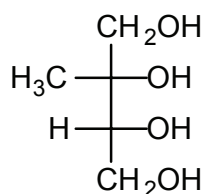
A serious global environmental problem is due to chemicals released by the Amazonian rain forest, but are the compounds previously unknown as claimed?

Thirty years ago chemists from Department of Organic Chemistry, NTH collaborated with chemists in Pakistan in order to solve the structure of an unknown compound isolated from a local variety of bindweed, *Convolvulus glomeratus*. Professor S. W. Shah (Fig. 1) from Sind came to Trondheim and spent nearly a year sponsored by NTNF, in order to resolve the structure.



Fig.1. Professor S. W. Shah, Greta Sommerschild and T. Ujar

At that time we had recently acquired our first useful NMR instrument, Varian A-60A, a marvellous instrument that opened new possibilities for natural product chemists. Quite soon we understood that the compound was sugar-like and we gave it the name Convolvitol, more systematically 2-C-methyltetritol. By synthesis it was shown to be the erythro diastereomer and later collaboration with Svante Brandänge in Sweden, it was identified using CD as belonging to the D-series and sugars. (Fig. 2)



D-Erythro

Fig. 2. Convolvitol, 2-C-methyl-D-erythritol isolated from bindweed, *Convolvulus glomeratus*.

The compound was synthesized by a first generation asymmetric synthesis starting with D-mannitol. This work was the basis of the Ph.D thesis of Steinar Hagen (Fig. 5). So, why bother with this old and solved problem now?

In 2004 an article appeared in the well recognized journal Science, reporting on huge amounts of aerosols collected in the atmosphere above the Amazonian rain forest. The compounds were identified by mass spectrometry as a diastereomeric mixture of 2-C-methyl tetritols, and claimed to be due to photo-oxidation of isoprenoids from plants. Furthermore, they were said to represent a huge global environmental problem since they occurred in large amounts (2 teragrams pr. year). Moreover, the compounds were claimed to be so far unknown. (Fig. 3)

The publication inspired us to return to the problem of 30-years back. Since Convolvitol contains two stereocenters, four stereoisomers are possible. If the aerosol consisted of enantiomers, this would be a conclusive evidence for it being of plant origin, i.e. formed by enzymatic processes, and not by photo-oxidation. Since the authors of the paper in Science did not isolate one single molecule, but only identified them by MS, there was no way they could identify their stereochemistry. This is crucial in order to identify them as being of plant origin or formed by photo-oxidation.

Formation of Secondary Organic Aerosols Through Photooxidation of Isoprene

Magda Claeys *et al.* Science Vol 303 20 February 2004, 1173-1174

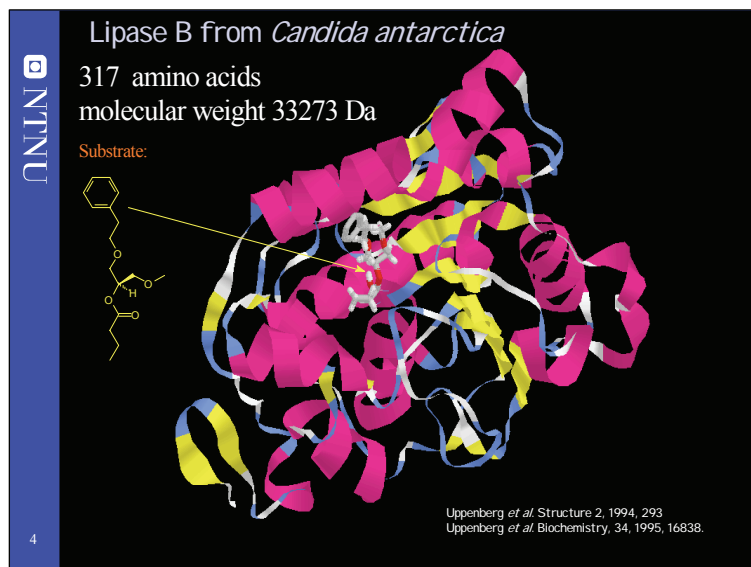
Detailed organic analysis of natural aerosols from the Amazon rain forest showed considerable quantities of **previously unobserved** polar organic compounds, which were identified as a mixture of two diastereomeric 2-methyltetritols: 2-methylthreitol and 2-methylerythritol.

"photooxidation of isoprene results in an annual global production of about 2 teragrams of polyols."

"they occur as a mixture of diastereomers (GC-MS of TMS ethers), consistent with a **non-enzymatic formation process**. Because the 2-methyltetritols are not of primary biogenic origin, they have to be considered as *secondary organic aerosol* components.

The 2-methyltetritols have, **to our knowledge, not been reported before.**"

Fig. 3. Extract of a paper in Science Vol 303, 20, February 2004, 1173-1174.



Using expertise in enzyme catalysis the Biocatalysis group has synthesized all four stereoisomers of Convolvitol by a combination of stereospecific oxidation and enzyme catalyzed kinetic resolution. (Fig. 4)

Fig. 4. Structure of lipase B from *Candida antarctica* with substrate modelled in active site.



Fig. 5. Skiers at "Linjestaffetten" 1979. 1. Row Harald Rønneberg, now research director Borregaard Synthesis, South Africa, Berit Johansen, now professor of Biology, NTNU, Karl Egil Malterud, now professor of Pharmacy, University of Oslo, Steinar Hagen, now Clavis Pharma, Oslo with son Bård, 2. row Swedish post doc., Petter Saksgaard and Liv Marit Henriksen, students, Vernon Parker, professor NTH, now professor, Utah State Univ., Thorleif Anthonson and Anne Fiksdahl, now both professors NTNU. Exhausted in front David Tauber, American post. doc. carotenoid group, in the back unidentified happy musician.

Thorleif Anthonson

Past pride - present problems. An automatic measuring system for monitoring heavy metal leakage from former mining areas

Copper pyrite (CuFeS_2) has for centuries been one of the most important minerals for the mining industry in Norway and several other places in the world. One of the most important mining areas in Norway was Løkken Verk, containing one of the greatest cuprous-pyrite deposits in the world. The mine was shut down in 1987, after a period of 333 years of mining industry.

Use of new technology introduced around the turn of the century resulted in a considerable rise in the production and at the same time also in the amount of waste material. Consequently, the pollution problems caused by acid rock drainage increased substantially. Former mining areas, which for centuries may have represented the basis of existence for a whole province, has in many cases gradually changed into considerable concerns, causing severe effects on several important river systems.

Even though considerable attention has been put on securing former mining and industry areas, leakage of heavy metals still takes place from such locations worldwide.

During 2005 the group of environmental chemistry and analytical chemistry at NTNU succeeded in installing new technology for automatically monitoring of environmental heavy metals in the field. Among others, a system was installed to monitor polluted river water impacted by zinc, iron and copper leaking from the former copper mine at Løkken Verk. Measurements were automatically carried out every half an hour for several months and compared to traditional sampled water samples measured by ICP-MS.

The obtained results attract attention, showing large variation in the different concentration within small time frames. Even more important, by combining results from traditionally measuring methods with results from the new automatically monitoring system it is possible to do speciation studies (Fig. 1) and extract unique information about the how the metals is bonded in the aquatic system, which is important since the toxicity of the metals depends on this. Further, continuous monitoring renders the possibilities to act immediately if accidental spills or short time pollution should occur.

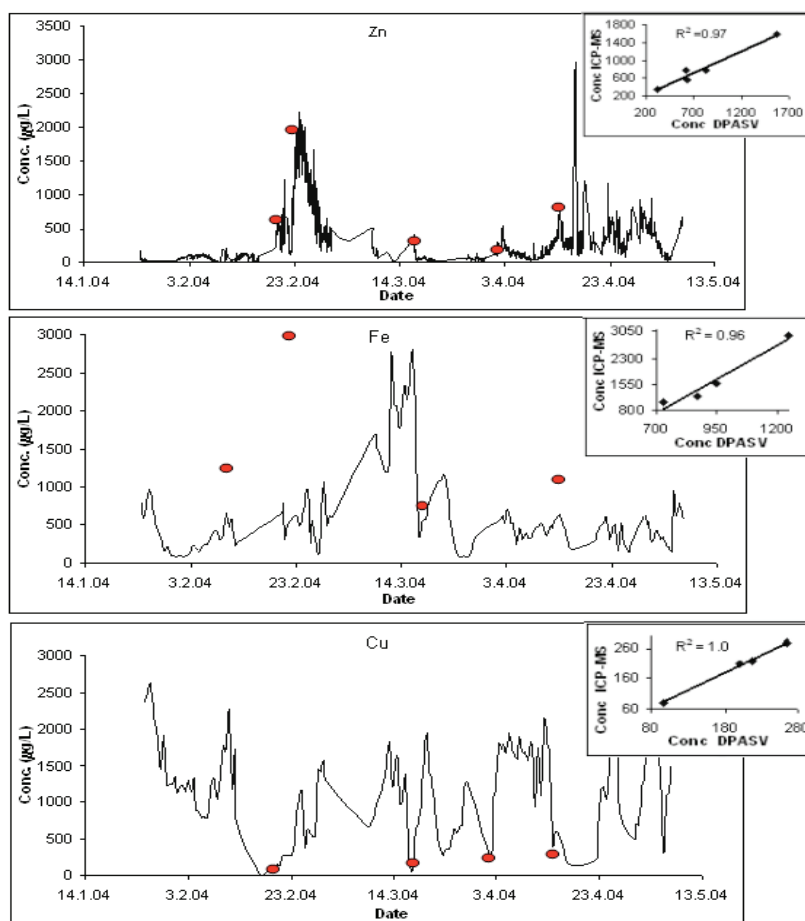


Fig. 1 Results from continuous monitoring

Monitoring of water quality is timely, especially in view of recent decisions in the European (Water frame work). The new method fulfills the needs for use in field, and opens up new possibilities for large scale water monitoring (valuable to the water policy in the European Union and other countries).

During the last part of 2005 a similar system was installed in the Yuyuan Hu river canal in Beijing in a joint research project with The China Institute of Water Resources and Hydropower Research (IWHR).

Øyvind Mikkelsen

Big aggregates - Small elementary units

Crystals are objects of mm to m size, classified by their morphology (monocline, tricline, rhombic, etc) however, all spectral properties can be described by small, periodic arrays of repeating entities, the 14 Bravais elementary crystal units (Fig.1)

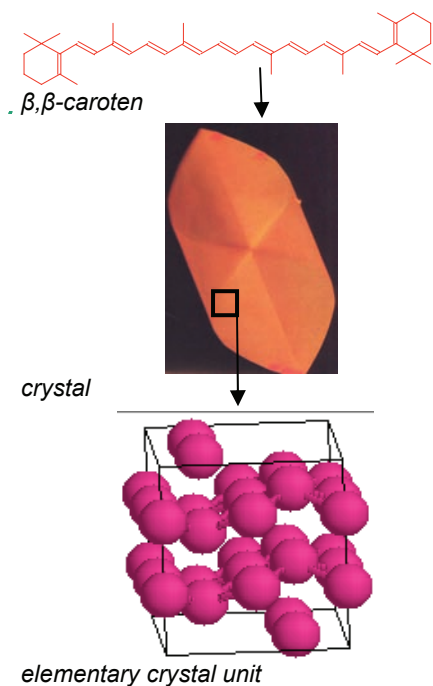


Fig.1. Crystal

Amphiphilic lipid molecules crystallize only with difficulty, but they easily self-assemble in water to aggregates (Fig. 2)

Aggregates are nm to μm objects, characterized by their topology (micelle, vesicle, bilayers) and arrangement (H- or J-aggregates). Properties have so far been derived from the entire assembly, formed by some few to hundreds of monomers.

We have found that both the spectroscopic and chiroptical properties of the carotenoid lysophospholipid aggregate can be described by a single, small entity: the basic aggregation unit. For the carotenoid lysophospholipid this basic unit represents an octamer. The possibility of basic units in aggregates has been recently postulated, without clear spectroscopic evidence.

Besides theoretical consideration hydrophilic carotenoids have a potential practical implication. Since nearly all carotenoids are lipophilic, their use as water-based colorants is considerably limited. Therefore, highly elaborated formulation procedures have been developed in industry to extend their use, e.g. for soft drinks.

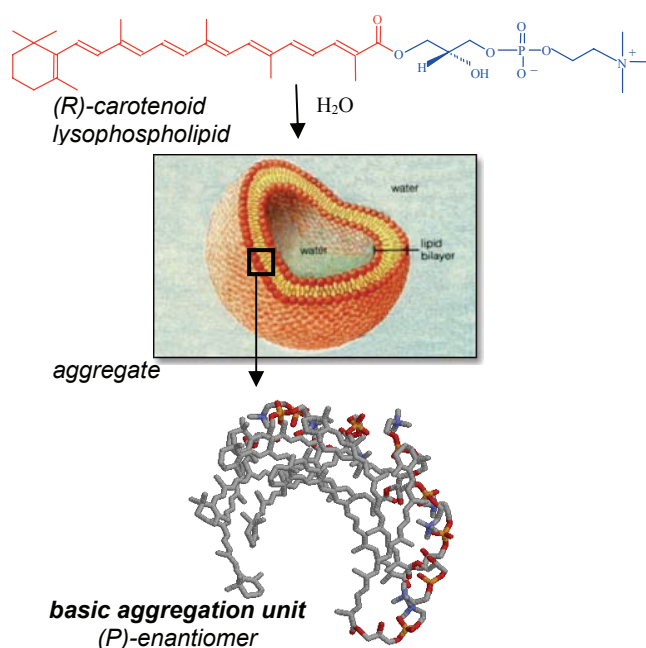


Fig. 2. Amphiphilic lipid molecules

We have combined hydrophobic carotenoids with hydrophilic groups. These new water-dispersible carotenoid derivatives do not need formulation, they formulate themselves by aggregation. This process locates the sensitive polyene chain to the aggregate's interior, the polar group to the aggregate's exterior. The polar-group membrane does not allow penetration of destructive compounds. Even after refluxing with HCl-solution, the aggregated carotenoid derivatives remain intact. The choice of the polar group is very important since they modulate the antioxidant properties (radical scavenging and singlet oxygen quenching). Hydrophilic carotenoids are, in addition, better antioxidants and one derivative is now clinically tested for the treatment of cardiovascular diseases.

BJ Foss, HR Sliwka, V Partali, C Köpsel, B Mayer, HD Martin, Z Bikadi, M Simonyi, Optically active octamer units in aggregates of a highly unsaturated, optical inactive carotenoid phospholipids, *Chem. Eur. J.* 2005, 11, 4103

TB Melø, HR Sliwka, SBB Mohamad, V. Partali, BJ Foss, ShH Abdel-Hafez, G Nadolski, H Jackson, SF Lockwood, Electron and energy transfer properties of carotenoid amphiphiles, in preparation

DA Lauver, SF Lockwood, BR Lucchesi, Disodium disuccinate astaxanthin (Cardax) attenuates complement activation and reduces myocardial injury following ischemia/reperfusion, *J. Pharmacol. Exper. Therapeutics* 2005, 314, 686

Vassilia Partali

X-ray absorption spectroscopy: an important tool in understanding catalytic mechanisms. Unveiling the role of copper in the selective catalytic reduction of NO_x over CuSAPO-5.

Collectively known as zeotypes, the open architectures adopted by aluminium phosphates (AlPO's) and zeolites contain pores with a wide range of diameters (3-20 Å). These microporous materials can serve as carriers in heterogeneous catalysis on which the active phase is finely distributed or by the introduction of species that alter the electronic, magnetic and catalytic properties of the material. The ability of CuSAPO-5 (Fig. 1) to catalyse the selective reduction of NO_x using propene as the reducing agent (SCR-HC) in an oxygen rich environment has been investigated. NO_x, a term representing the nitrogen oxides, is part of the waste gases emitted from combustion processes in both stationary and mobile sources. NO_x is a potent pollutant because it reacts with sunlight in photochemical processes to produce smog and acid rain making it a serious environmental challenge globally.

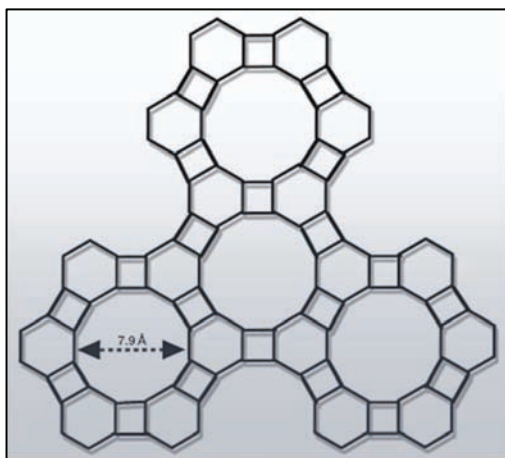


Fig. 1. The SAPO-5 large pore framework with one-dimensional channels yielding a large inner surface.

The mechanism for selective catalytic reduction of NO_x with hydrocarbons in an oxygen-rich atmosphere is still being debated. Several studies have been carried out on several aspects of the contributing factors such as the role of the zeolitic system versus the role of an introduced metal including its preferred site and redox properties. One mechanism proposed for selective nitric oxide reduction is the redox mechanism. This utilises the reversible valence states of copper in this material visualised in Fig. 2 showing the steps involved in this reaction.

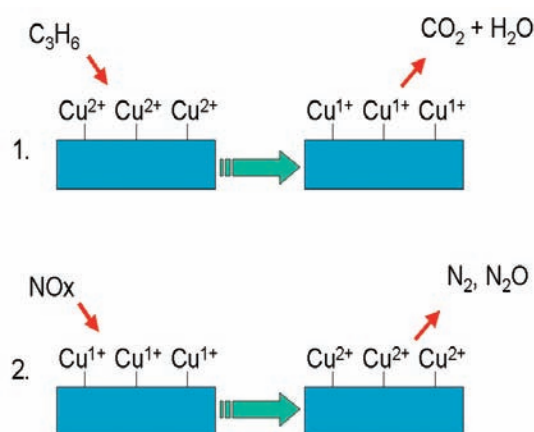


Fig. 2. Proposed red-ox mechanism for the reduction of NO_x over copper materials.

The major part of the characterisation of the system is by x-ray absorption spectroscopy using synchrotron radiation to investigate the copper environments. The objectives for using X-ray absorption spectroscopy for studying metal incorporated aluminium phosphates are many. This technique is an element specific local probe, which means we can select our metal of interest and study its local environment including coordination, valence state and bond distances.

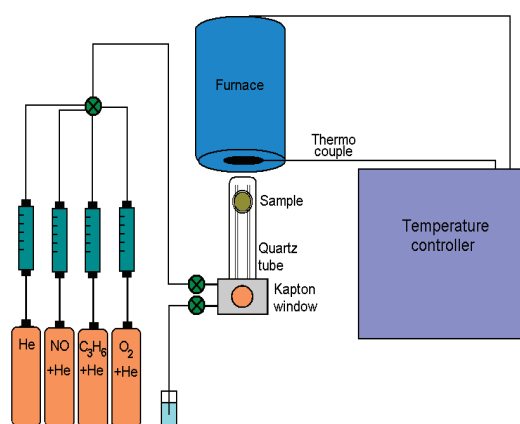


Fig. 3. In-situ setup used for pre-treatment of samples prior to XAS data collection.

In-situ cell

There is considerable interest in investigating the mechanism, and particularly the role of copper in CuSAPO-5 during reduction of NOx. X-ray absorption and especially the x-ray absorption near edge region (XANES) gives information about the valence state of copper, which can be followed using an in situ cell (Fig. 3). The local environment around copper can be monitored during a stepwise treatment of the catalyst in the reacting gases. The redox behaviour of copper in the CuSAPO-5 system during selective catalytic reduction of NOx with propene (SCR-HC) is shown below. The catalysts were treated in stages with the components (helium, NOx, propene) of the SCR-HC process while monitoring the copper valence state.

XANES

The x-ray absorption near edge (XANES) region of the XAS spectra yields information about valence state and geometric and electronic properties. The position of the edge and specific features before and after the edge serves as a fingerprint for elucidating structural information. This is particularly useful for copper compounds as seen in the Figure below. XAS data was collected at BM01 (SNBL) and BM26 (DUBBLE) at the ESRF.

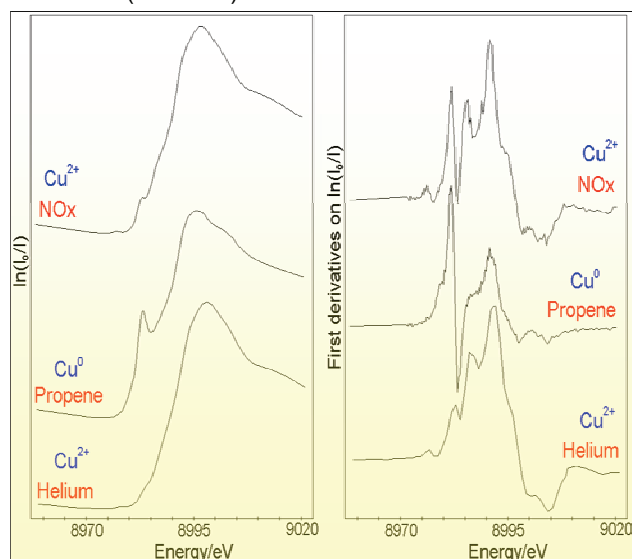


Fig. 4. Normalised and first derivative XANES spectra for CuSAPO-5 treated stepwisely in the gas components for the selective catalytic reduction of NOx with propene (SCR-HC).

EXAFS

Through data refinement information about the nearest neighbours of the absorbing atom can be obtained. This includes number and type of backscatterer and also thermal disorder of the bonds. X-ray absorption spectroscopy has proven especially suited for studying catalytic systems provided that the active metal in question can be studied using this technique. XAS is extremely versatile in terms of the nature of the sample and the experimental setup also allows for the use of in-situ cells in which both the temperature and

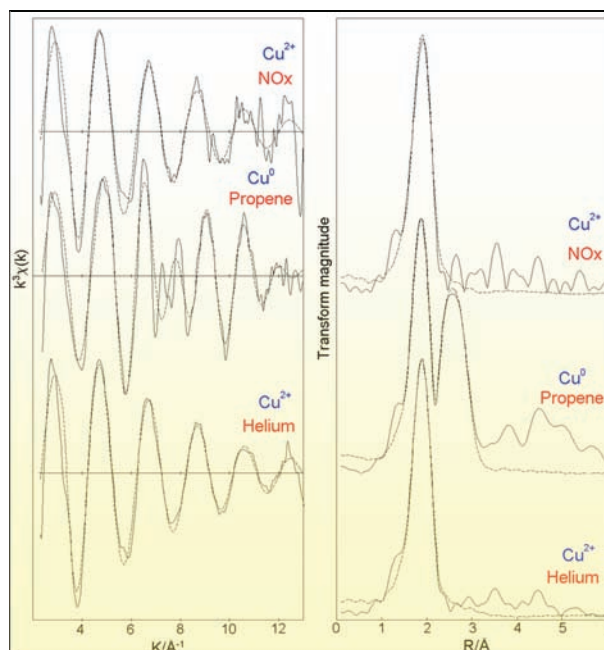


Fig. 5. Experimental (—) and calculated (---) Fourier filtered (1-25) k^3 -weighted EXAFS and its Fourier Transform for CuSAPO-5 treated stepwisely in the gas components for the selective catalytic reduction of NOx with propene (SCR-HC).

gaseous environment can be altered to simulate “real conditions” of a working catalyst.

The addition of silicon to the synthesis of CuAPO-5 to yield CuSAPO-5, has a negative effect on the activity towards selective catalytic reduction of NOx. In-situ XAS studies of a low copper and silicon content CuSAPO-5 show that a small fraction of copper is reduced to copper(I) by helium, and that metallic copper is formed in propene. Unlike the CuAPO-5 samples metallic copper is redispersed and subsequently reoxidised and copper(I) is reoxidised by NOx. The red-ox mechanism is therefore a possible route for reducing NOx over CuSAPO-5, in addition to acid sites. CuSAPO-5 with high copper and silicon contents is inactive for the SCR deNOx process which can be explained in terms of pore blocking and formation of copper(II) oxide during propene and NOx treatments.

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Karina Mathisen and David G. Nicholson

A description of active transport in biological systems

This year the research group in physical chemistry succeeded to find a theoretical description of a 40 year old problem: How can we understand that chemical energy, which has no direction (is a scalar) can lead to a directed (vectorial) transport of ions?

Such a transport takes place in many biological systems where chemical energy (food) is converted to work. The transport of ions takes place uphill against a concentration difference, and therefore requires work. In the process energy is dissipated as heat.

The group has found a description of the events on a statistical level, by extending thermodynamic equations of transport to this mesoscopic level. At this level molecular fluctuations play a major role. The theory developed to describe these processes, is called mesoscopic non-equilibrium thermodynamics. It is surprising to see how much it resembles a theory on the macroscopic level. We now hope that similar problems in biology also can find an interesting solution.

The figure illustrates the Ca-Mg-ATPase. This protein is responsible for transport of calcium in muscles, by means of the reaction of adenosintriphosphate to adenosindiphosphata. This system was used to develop a theory for active transport.

S. Kjelstrup, J.M. Rubi, and D. Bedeaux, Active transport: Kinetic description on thermodynamic grounds, *J. Theoretical Biology*, **234** (2005) 7-12)

S. Kjelstrup, J.M. Rubi and D. Bedeaux, Energy dissipation in slipping biological pumps, *Phys. Chem. Chem. Phys.* **7** (2005) 4009-4018

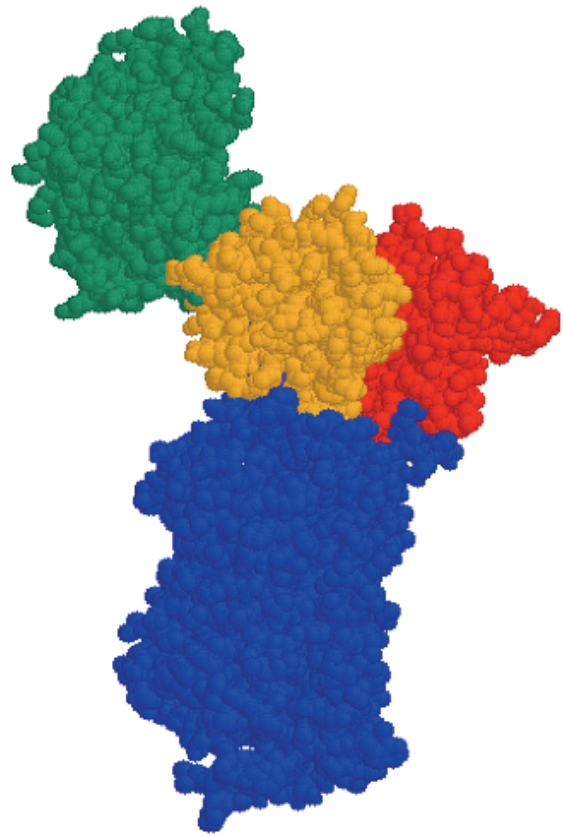


Fig. 1 Ca-Mg-ATPase

Signe Kjelstrup

Large electronic structure calculations and applications to the first carbon nanoring

In 2003 Kawase et al. [1] reported the synthesis of the first nanorings. In particular they synthesized one complex formed by the inclusion of hexamethylbenzene in 6-cycloparaphenylacetylene (see Fig. 1). Since then a family of similar compounds have been obtained by that group as molecular recognizers of fullerenes. Quantum Chemistry can play a fundamental role in explaining the properties of these complexes, provided that the chosen theoretical method is able to give a correct picture of the different types of attractive forces that can explain the formation of the complex, namely electrostatic interactions, charge transfer and van der Waals dispersion.

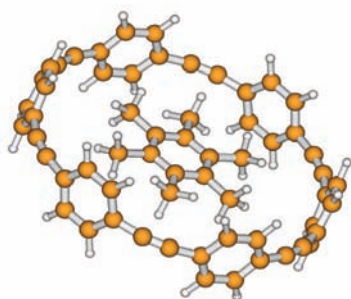


Fig. 1. The structure of the inclusion complex of HMB in 6-CPPA

From the theoretical point of view, the computationally cheaper methods like density functional theory (DFT) based methods can describe simple electrostatic as well as charge transfer interactions, but are not at the moment able to describe weak van der Waals forces. We have recently shown [2] that the decomposition of two electron integrals by means of Cholesky decomposition techniques facilitates the algorithm for electronic structure calculations of large molecular systems, making it possible to calculate the interaction energy as well as many other molecular properties [3]. In these calculations [4] we use second order Møller Plesset perturbation (MP2) theory. The information so obtained allows understanding the nature of the bonding in this system.

Quantum chemical calculations at both Hartree Fock and B3LYP levels predict the complex to be dissociative. Since DFT methods can in general give account of electrostatic interactions –and also Hartree Fock- possible electrostatic interactions do not suffice to explain the experimental bonding. On the other hand, the B3LYP functional has been extensively used to study supramolecular systems that remain bound by effect of charge transfer processes. This is identified in many cases by inspection of HOMO and LUMO orbitals. Anyway, strictly speaking, molecular orbital are not physical observables and, in fact, they are only determined until any unitary transformation not mixing the mutually orthogonal occupied and virtual subspaces. Instead we have preferred to study the electron density, which is an invariant physical observable.

In Fig. 2 we have represented the electron density for 6-CPPA (2a), HMB (2b) and the inclusion complex (2c), as well as the difference (2d) between the density of the complex and the sum of the densities of the two fragments, which represent the charge transfer, all calculated using the B3LYP parameterization of the density functional. It is observed that inter-fragments charge transfer occurs to an absolutely negligible extend and, accordingly, it should be disregarded as responsible of the bonding. Therefore, intermolecular bonding can only be explained in terms of dispersion interactions.

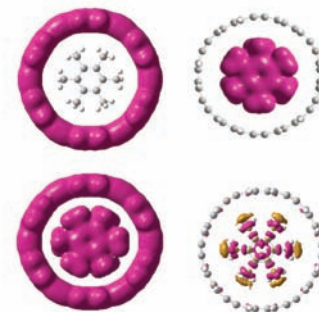


Fig. 2. Isodensity surfaces of HMB (a), 6-CPPA (b), 6-CPPA•HMB (c), and variation of density upon complexation (d).

Summarizing, our theoretical studies show that in the 6-CPPA•HMB inclusion complex, HMB is placed in the centre of the horizontal symmetry plane of the 6-CPPA ring with the methyl groups pointing to the acetylene bridges of the host cycle, in agreement with the experimental evidence and with previous semiempirical studies. The most important issue is the fact that bonding is mainly due to van der Waals dispersion forces and, consequently, MP2 is the cheapest theoretical model able to correctly describe the electronic structure of molecular systems of this kind.

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Support

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Henrik Koch

Pioneering work on a pioneer in chemistry.

In 2005 the Department of Chemistry at NTNU could celebrate a Ph.D completed within history of chemistry- the very first in Norway. The candidate was Annette Lykknes. Parts of the results have been published in the most prestigious journal existing within this field, namely *Isis*. This project is an example of successful interdisciplinary collaboration at NTNU, namely between the Department of History (Anne Kristine Børresen) and the Department of Chemistry (Lise Kvittingen).

In this project the Norwegian chemist Ellen Gleditsch (1879-1968), who became Norway's first authority on radioactivity and Norway's second female full professor was studied. Gleditsch travelled in 1907 as a young, hopeful and ambitious pharmacist to Marie Curie's laboratory in Paris.



Ellen Gleditsch in her laboratory

There she spent five years first acquiring knowledge and practical skills and later participating in important debates at the beginning of this field (radioactivity was discovered in 1896), where questions abounded answers. The cosmopolitan (and slightly feminine) atmosphere of Curie's lab was to Gleditsch's liking, many of her acquaintances from this period were to last her lifetime. Together with women in the Vienna Radium Institute and in Manchester, working under Ernest Rutherford, a "network of women in radioactivity," was established, although it was never formalised.

Always internationally oriented, Gleditsch worked at the Sloane Physics Laboratory at Yale University (1913-14), had several stays in Vienna and frequently returned to Paris throughout her career. From 1926 to 1929 she was president of the International Federation of University Women; her network thus included all academic fields.

Despite being internationally acknowledged and having an extensive personal and scientific network, she was never fully appreciated in the Norwegian scientific milieu. This culminated in 1929 during the controversy around her professoral appointment. Gleditsch had cultivated international networks more than national, but it was in Oslo she was to create a research and teaching laboratory of radiochemistry. Together with a heavy teaching load and a tight economic period this was challenging. It was first under her student, Alexis Pappas, who was appointed professor a decade after Gleditsch retired in 1946, that a research group of radiochemistry started to grow properly, as financial support improved and the field benefited from a wave of new discoveries and inventions in the field which now was renamed "nuclear chemistry." Whether Gleditsch succeeded in making a research and teaching laboratory of radiochemistry during her career can be discussed, but through her student, Pappas, she definitely had success by proxy.

Lise Kvittingen

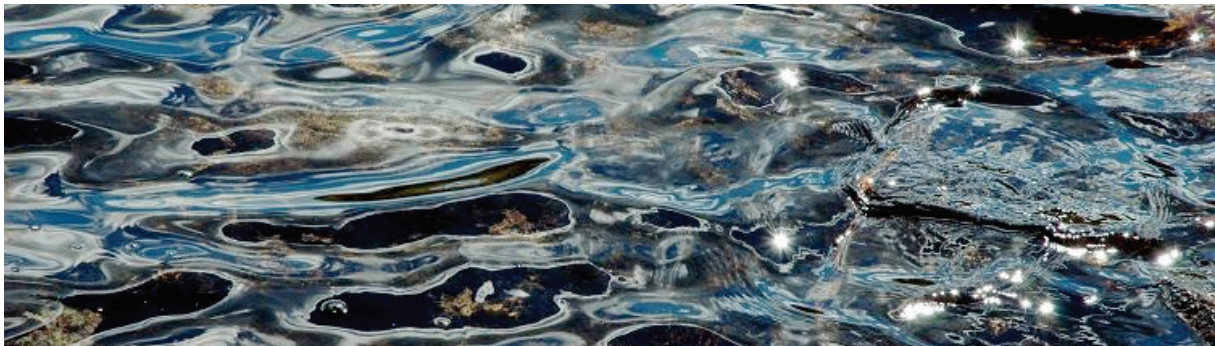
Investigation of selected natural and anthropogenic radionuclides in reindeer (*Rangifer Tarandus Tarandus*) and lynx (*Lynx Lynx*).

PhD thesis by A. L. Skuterud

A range of dietary, physiological and environmental factors influencing transfer and long-term behaviour of radionuclides in reindeer and lynx were investigated. The radionuclides concerned were ^{137}Cs and ^{90}Sr from anthropogenic sources (nuclear weapons fallout and the Chernobyl reactor accident), and ^{210}Pb and ^{210}Po from the natural radioactive decay of uranium. Part of the thesis dealt with feeding experiments where reindeer were given shorter-lived radioactive isotopes of Cs and Sr to study the turnover of ^{137}Cs and ^{90}Sr in the animals and transfer to the offspring. Furthermore the concentrations of the four radionuclides in soils and pasture plants in two reindeer herding districts and

the transfer to grazing reindeer were studied and the corresponding radiation doses to population groups were estimated. The ^{137}Cs originating from the Chernobyl accident continues to be a problem in Norway after almost two decades. An additional study dealt with ^{137}Cs in the muscle of 747 lynches killed in Norway during the period 1986-2001 and its dependence of geographical deposition pattern, time after fallout, age, and extent of reindeer grazing area.

Lavrans Skuterud:



Behaviour of some nutrients and heavy metals in Scandinavian coniferous forest affected by human activity

Dr.Scient. thesis by L. K. Grønflaten

Modern forestry practices may disturb the chemical balances in the soil and hence the uptake of essential elements as well as harmful metals in forest trees and understorey vegetation. In this work the behaviour of Mg, K, Ca, Cr, Mn, Cu, Zn, and Pb in surface soil and forest plant species following different methods of forest clear-cutting, short-term liming, and vitality fertilization was investigated. The fieldwork was carried out at Birkenes and Åmli, southern Norway and Asa, southern Sweden. The behaviour of the nutrient elements K, Ca, and particularly Mn in the soil was considerably affected by clear-cutting, and so was also the uptake in the forest grass *Deschampsia flexuosa*. The changes in

the other elements were less pronounced. Liming and fertilisation caused appreciable changes in the behaviour of the metals Mn, Cu, Zn, and Pb in the soil and some understorey plant species in a Scots pine ecosystem. In a laboratory study four different chemicals (NH_4OAc , NH_4NO_3 , dilute HCl, and EDTA) were tested as means of extracting the plant-available fraction of the above trace metals in forest soil, but none of the extractants showed satisfactory correspondence with the levels observed in the forest plants.

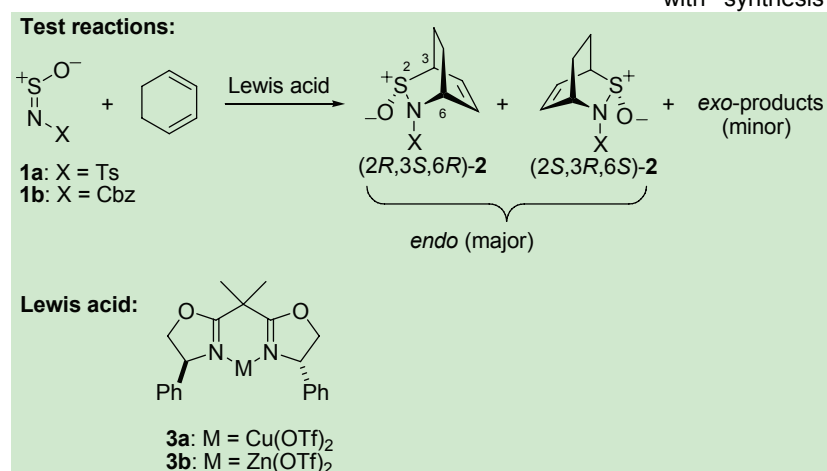
Lena Kjølbi Grønflaten

Catalytic Enantioselective Hetero-Diels-Alder Reactions of N-Sulfinyl Dienophiles

PhD thesis by M. M. Endeshaw

The Diels-Alder (DA) and hetero-Diels-Alder (HDA) reactions constitute an extremely useful set of reactions for stereoselective synthesis. In this project the main objective was to develop catalysts for the asymmetric HDA reaction between N-sulfinyl dienophiles (**1**) and dienes. The resulting heterocyclic products can be further transformed into synthetically useful derivatives, e.g. homoallylic amines and vicinal amino alcohols, by well established techniques.

A series of chiral Lewis acids were screened as promoters for the asymmetric HDA test reaction of N-sulfinyl dienophiles **1a** and **1b** with 1,3-cyclohexadiene shown in scheme 1. The best results were obtained by using stoichiometric amounts of Lewis acids **3a** and **3b** providing the endo adducts **2a** and **2b** in good enantioselectivities (90 – 98% ee), diastereoselectivities (>90% de), and yields (63-85%).



Scheme 1. The test system: HDA reactions of N-sulfinyl dienophiles **1a** and **1b** with 1,3-cyclohexadiene.

Attempts to perform the test reactions with catalytic amounts of the Lewis acids gave rather disappointing results. A distinct drop in de and ee was observed with 10 mol % loading of either **3a** or **3b**.

In order to increase the catalytic turnover of the two Lewis acids, two strategies were tested: i) Screening of a series of N-sulfinyl dienophiles **1** in the asymmetric HDA reactions, and ii) screening of additives assumed to assist the release of the chiral catalyst from the HDA adducts. The N-sulfine survey did not point out any better N-sulfinyl dienophiles for the asymmetric HDA reaction. However, the second strategy proved to be more promising. The optimized system containing 10 mol % of either **3a** or **3b** and 100 mol % trimethylsilyl trifluoromethanesulfonate (TMSOTf) gave yields and stereoselectivities comparable with the stoichiometric reactions described above. With the optimized system in hand several cyclic and acyclic dienes were tested. In general, the copper catalyst **3a** and N-sulfine **1b** was found to be most efficient (54->90% de, 30-98% ee).

Application of this methodology was showcased with synthesis of i) (2*R*,3*S*)-N-benzoylphenylisoserine methyl ester, a derived side chain of the antitumor agent Paclitaxel (Taxol), and ii) (3*aR*,6*aS*)-3,3*a*,4,6*a*-tetrahydrocyclopentaoxazol-2-one, a precursor of the C-ring in the antitumor marine sponge alkaloid Agelastatin A.

The absolute configuration of the HDA adducts were determined either by X-ray analyses (in cooperation with professor Lars Kristian Hansen, University of Tromsø) or by chemical correlation with known compounds.

The project was supported by the Norwegian Research Council (grant 140593/431) under supervision of associate professor Odd R. Gautun. Dr Endeshaw is currently working as a research scientist at Borregaard Ind. Ltd., Department of Synthesis R&D in Sarpsborg.

Molla Mellese Endeshaw

Synthesis and physical properties of hydrophilic carotenoid derivatives

PhD thesis by B. J. Foss, February 2005

The thesis describes the synthesis of new water-dispersible carotenoid derivatives and the investigation of the physical and biological properties of these compounds.

UV-VIS spectroscopy revealed that most of the water-dispersible carotenoids show hypsochromic λ max shifts upon addition of water, which may be a result of H-aggregate formation. The aggregates are disrupted into monomers when organic solvents such as methanol, are added to the solutions.

The data from the surface tension measurements show that these new surfactants all reach their critical micellar concentration (cmc) at relatively high concentrations, while lowering the surface tension markedly. The hydrodynamic radius of their aggregates could be determined from dynamic light scattering measurements.

The biological activity of the carotenoid lysophosphocholine (**1**) was investigated by spin trap-DEMPO EPR spectroscopy, and was shown to be a potent aqueous phase direct scavenger of superoxide. Over 90% of the superoxide anion was scavenged.

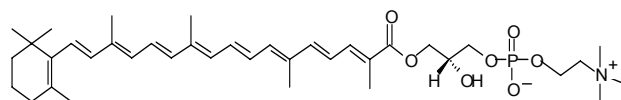


Fig.1 Carotenoid lysophosphocholine (**1**)

The antioxidant properties of compound **1** were investigated by laser flash photolysis. The collision between the sensitizer and the carotenoid either

lead to energy- or electron-transfer, and the ratio of the reaction change with solvent polarity. The carotenoid lysophosphocholine compound **1** exhibit supramolecular self-protecting properties in water due to their aggregate formation where the sensitive polyene chain is placed into the interior of the aggregate.

The optical activity of **1** was investigated by CD spectroscopy. It was found that compound **1** was optical inactive in the monomer form (in methanol). When dissolved in water, a chiral aggregation was induced. Based on molecular mechanics calculations, an enantiomeric oligomer composed of approximately eight monomers as the basic unit of the aggregates was proposed.

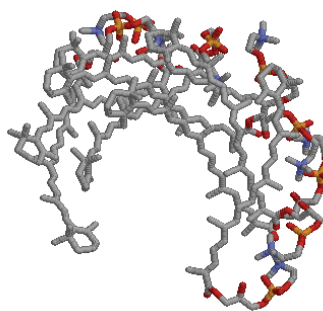


Fig. 2. Calculated basic aggregation unit of the optical active carotenoid derivative **1**

Vassilia Partali

X-ray absorption spectroscopic studies on active metal sites in zeotypes during the selective catalytic reduction of NO_x with propene in an oxygen rich atmosphere.

PhD thesis by K. Mathisen

This thesis is concerned with the synthesis and characterisation of CuAPO-5, CuSAPO-5 and also copper ion-exchanged SAPO-5, SAPO-11 and ZSM-5. The ability of these materials to catalyse the selective reduction of NO_x using propene as the reducing agent (SCR-HC) in an oxygen rich environment has been investigated. NO_x, a term representing the nitrogen oxides, is part of the waste gases emitted from combustion processes in both stationary and mobile sources. NO_x is a potent pollutant because it reacts with sunlight in photochemical processes to produce smog and acid rain making it a serious environmental challenge globally.

Samples have been characterised by in-house methods like x-ray powder diffraction for phase determination, surface measurements and scanning electron microscopy for particle morphology (Fig.1).

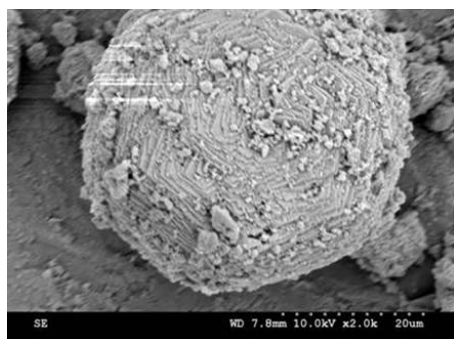
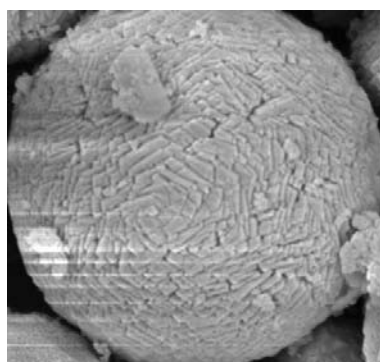


Fig. 1 Showing particle shape and size of CuAPO-5 (top) and CuSAPO-5 (bottom).

By using X-ray absorption spectroscopy we can select our metal of interest and study its local environment including coordination, valence state and bond distances. The structure of CuAPO-5 has

also been investigated by synchrotron x-ray diffraction data using the Rietveld method to elucidate the effect that incorporated copper(II) has on the overall AlPO₄-5 lattice. In this work we have combined x-ray absorption spectroscopy as a local probe, with the bulk technique x-ray powder diffraction because these techniques together give a broader view of the material (Fig. 2).

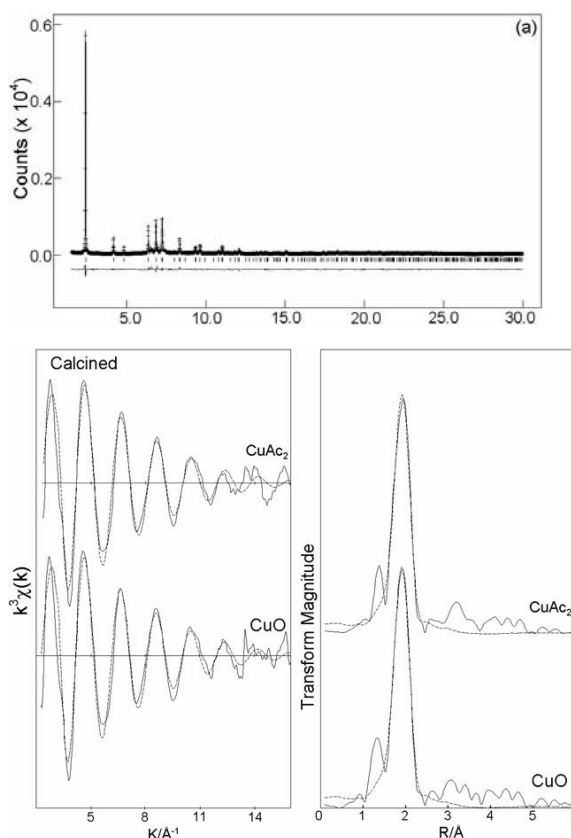


Fig. 2 Rietveld refinement (left) and Fourier Transformed EXAFS (right) of CuAPO-5 material.

The motivation for introducing copper into the aluminium phosphate number 5, AlPO₄-5 stems not only from the interesting properties of these materials, which include molecular sieving properties, shape selectivity and thermal stability, but also the ability of copper materials to catalyse the selective catalytic reduction of NO_x.¹⁻⁴ We have resolved the issues regarding the change in copper environment upon calcination (Fig. 3) and also the issue of the choice of copper source.⁵



Fig. 3 As-synthesised and calcined CuAPO-5, colour change indicative of change in copper environment

A natural extension to our studies on CuAPO-5 was to synthesise CuSAPO-5.⁶ Introducing silicon into the lattice gives rise to an additional property – a net negative charge localised on an oxygen atom. Calcination causes protonation which produces a hydroxyl group. These groups function as a Brønsted acid site. There is considerable interest in investigating the mechanism, and particularly the role of copper in CuAPO-5, CuSAPO-5 and the ion-exchanged analogues during reduction of NOx.⁶ X-ray absorption and especially the x-ray absorption near edge region (XANES) gives information about the valence state of copper, which can be followed using an in situ cell. The in-situ experiment was set-up to imitate the conditions of the catalytic measurements, and to monitor the copper valence state during the different stages of reaction (Fig. 4).

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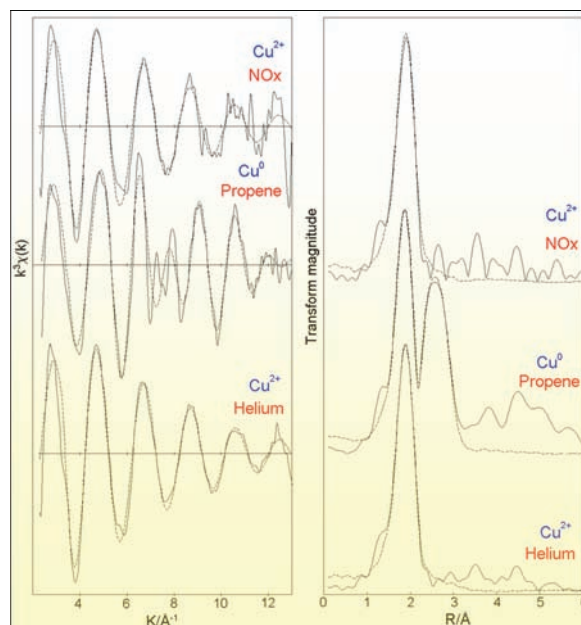


Fig. 4 Experimental (–) and calculated (–) Fourier filtered (1-25) k^3 -weighted EXAFS and its Fourier Transform for CuSAPO-5 treated stepwisely in the gas components for the selective catalytic reduction of NOx with propene (SCR-HC).



Karina Mathisen

ESRF

This photo was taken in June 2005 by German professional photographer Peter Ginter (<http://www.peterginter.de/index1.html>). The picture was taken early in the morning before the sunrise.

It was taken with a Canon EOS-1DS MARK II with a focal length of 15 mm at a speed rating of 200, aperture F13.

For more details concerning the hour and conditions of weather when the picture was taken, contact Mr Andreas Freund (freund@esrf.fr) who initiated this project of artistic photographs.

Courtesy of the ESRF

Open days UKA 2005. One of the largest student recruiting arrangements at the University

Hundreds of excited scientists *in spe* visited our department.

Arrangement by PhD students Kristina Strasunskiene and Anders Riise Moen, technician Kjersti Ljones and Dr. Scient. Elisabeth Jacobsen

1400 junior high school pupils and college students visited NTNU during Open Day 10th of October. Ideally we, as student recruiters, hoped that all of them would visit our department. However, we had our hands full guiding and advising the nearly 150 boys and girls from Lade, Oppdal, Vikhammer, Malvik and Ringve who paid us a visit. Citizens of Trondheim were invited to visit NTNU Sunday 9th of October, and 50 of them came to our department.



Pupils from Oppdal were fascinated by all the different chemicals.

On entering the second floor in the Realfagbygget, our visitors were shown an exhibition of old colourful chemicals from the last century, samples of war gases, natural products and instruments used in scientific research. All of these historical items were excellent illustrations of chemistry, the science of MOLECULES.

Dr. Scient. Elisabeth Jacobsen wished our visitors welcome by emphasizing the importance of knowing about the chemistry of nature and our bodies; these being the most important chemical "factories" in the world! The importance of a continuing search for new pharmaceutical drugs from existing natural products over last decade was mentioned along with the development of materials and analytical techniques within modern chemistry. Before the visitors were allowed to take a closer look at the different chemicals and instruments they were informed about chemistry bachelor- and master courses at the University.



A few samples of the 2795 organic compounds called "Præparatsamlingen", used to visualise organic compounds in chemistry classes at NTNU from 1911. Some of the chemicals are still in use for the same purpose!

This general introduction was followed by a guided tour in the Realfagbygget. In the analytical chemistry laboratory PhD student Kristina Strasunskiene informed about electrochemical methods and the possibilities of field surveillance of heavy metals in water. PhD student Anders Riise Moen informed about organic synthesis of pharmaceutical drugs and some of the important analysis methods used in organic synthesis.

We also had to answer a lot of questions: What exactly is chemistry research? Is it difficult? Which jobs can I get? Do I need to study mathematics in order to be a good chemist?

This arrangement is an excellent way of presenting the research and education at our department for pupils and college students who are interested in chemistry and science.

Hopefully, we will meet some of our visitors as NTNU students next Autumn!

*Elisabeth Jacobsen
Photographs by Thorleif Anthonson*

The ECOS 2005 Conference



The ECOS 2005 conference is part of a series of international meetings that focus on modern aspects of thermal science with particular emphasis on engineering thermodynamics.

The name ECOS is the acronym for Efficiency, Costs, Optimization and Simulation of energy conversion system, keywords that best describe the contents of the papers presented at these meetings.

The environmental impact of these systems is implied by the name too. ECOS means "home" in the Greek language. Indeed, many participants have found in this series of conferences an appropriate "home" for discussing their ideas and work progress.

The Conferences have been held all over the world (Rome, Beijing, Cracow, Istanbul, Tokyo....) and was held this year in Trondheim, under the leadership of Prof. Signe Kjelstrup.

There were 320 participants from 36 countries. Supporters were Statoil, Hydro, Norske Skog, Gassnova, Enova, the Norwegian Research Council, ASME, IEA and the Gas Technology Centre, NTNU – SINTEF.



Flag parade for the 36 country participants

The Proceedings of the conference are obtainable from the Institute office.

The Conference presents five key note talks:

Commemorating Prigogine, de Groot and Mazur
(Prof. O. Arnas)

CO₂ – from problem to business opportunity
(Dir. T. Sundset, Statoil)

Computational Fuel Cell Engineering: Challenges and Opportunities
(Prof. N. Djilali)

Climate change and energy policy: The importance of sustainability arguments
(Prof. Roland Clift)

Process integration: Current status and Future Potential
(Prof. Robin Smith)



R7 plenum Key note talk

Special Conference sessions:

Industrial ecology for energy technology
(responsible: Prof. E. Hertwich)

Process integration as applied to large energy users and producers
(responsible: Prof. T. Gundersen)

Nanoscale non-equilibrium thermodynamics
(responsible: Prof. M Rubi)

Renewable energy systems
(responsible: T. Sundset)

Signe Kjelstrup

Scientific publications

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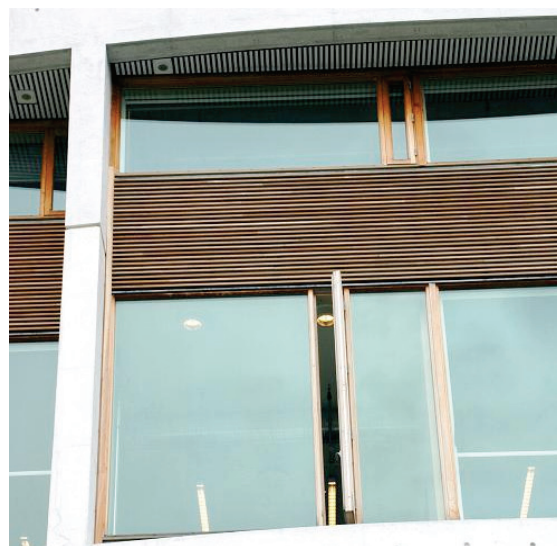
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Weck, Gaetan; Åstrand, Per-Olof. Interaction and Equalization Models to Calculate Molecular Dipole Moments and Polarizabilities. *Lecture Series on Computer and Computational Sciences*; 2005

Zvolinschi, Anita; Johannessen, Eivind; Kjelstrup, Signe. The second law optimal operation of a newsprint paper drying machine. *Proceedings of ECOS 2005*; 2005

Åstrand, Per-Olof. Computational Molecular Science: Hybrid Classical-Quantum and Force Field Methods. *Lecture Series on Computer and Computational Sciences 4A*; 2005



Honours, Extracurricular activities, Participation in courses, conferences, lectures and study visits

B. Alsberg

Conference "Det 17. Norske Kjemometrisymposium", Geilo, Norway, March 14 - 16, 2005. Lectures on: "Hyperspectral imaging in microarrays" and "SciCraft: An open source data analysis tool".

Bioinformatics Forum for Young Scientists, Randsvangen, Norway, April 15 - 17, 2005. Lecture on: "Drug Comparison Based on Quantum Topology and Inductive Logic Programming"

European Science Foundation (ESF) Training Course, Microarray Gene Expression Analysis - Power and Potential of Standardisation; May 23 - 27, 2005.

Poster presentation on: Medical Technology in cardiovascular disease: The use, development and integration of microarray technology, statistics and computational biology on definition of a "Life style algorithm" to be employed in chronic disease prevention, diagnosis and therapy.

9th Scandinavian Symposium on Chemometrics (SSC9), Reykjavik, Iceland, Aug. 22 - 25, 2005. Lectures on: "How Octave can replace Matlab in Chemometrics" and "Chemometric Analysis of Microarrays".

2nd ESF Functional Genomics Conference "Functional Genomics and Disease"; Sep. 6 - 10, 2005.

Poster presentation on: Definition of a "lifestyle algorithm" to be used in chronic disease prevention, diagnosis and therapy.

Course in "Microarray data analysis", University of Tromsø, Norway, Oct. 2005.



E. Anderssen

NBS Winter Meeting and Contact Meeting, Tromsø, Norway, Jan. 13 - 16, 2005.

Lectures on: Design of Microarray Time Series Experiments" and "Design and Analysis of microarray Time Series Experiment".

Poster presentation on: Effects of choice and dose of dT blockers in cDNA microarray experiments.

Course in "Microarray data analysis", University of Tromsø, Oct. 2005.

Lecture at Norwegian Microarray Consortium, ESF course, Trondheim, Norway.

Lecture at Norwegian Microarray Consortium, ESF course, Bergen, Norway.

International symposium; Dec. 9 - 10, 2005.

Co-author on lecture on: Gene expression profiling of orthotopic rat bladder cancer model.

T. Andreassen

Conference "20. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 13 - 16, 2005.

T. Anthonsen

Member of Editorial Board:
Journal of Molecular Catalysis, B Enzymatic Biocatalysis and Biotransformation.

Chairman Management Committee
COST Action D25. Applied Biocatalysis, Stereoselective and Environmentally Friendly Reactions Catalyzed by Enzymes. 22 Member Countries

Conference 20th Norwegian Organic Chemistry Wintermeeting, Skeikampen, Norway, Jan. 13 - 16, 2005.

Lecture on: Chemo-enzymatic synthesis of enantiopure 2-C-methylthreitol and 2-C-methylerythritol Meeting

Poster presentation on: Synthesis of chiral building blocks from acetovanillone.

Poster presentation on: Synthesis of enantiopure acrylates and their use in alkene metathesis.

COST, Chairman Management Committee, Fefor, Norway, Feb. 25 - 27, 2005.

Jan Bakke Seminar, NTNU, Trondheim, March 11, 2005.

Board meeting European Federation of Biotechnology, ESAB, Brussels, March 18 - 20, 2005.

Meeting KOSK, The Research Council of Norway, Oslo, May 2 - 3, 2005.

Meeting, Management Committee, Chairman, Mid-term evaluation, Delft, Netherlands, July 7 - 9, 2005.

Conference "Industrial Biocatalysis in Pharmacy and Fine Chemistry", Nimes, France, Sep. 8 - 11, 2005. Poster presentation on: Synthesis of chiral building blocks from acetovanillone.

Opponent Doctoral Thesis of Rong Liu, "Enzymes as Catalysts in Synthesis of Enantiomerically pure building Blocks", KTH Stockholm, Sweden, Sep. 30, 2005.

Conference "Organisk kjemisk høstmøte", Oslo, Nov. 11, 2005.

Meeting "Bioprospektering i norsk natur - muligheter for industriell utnyttelse", NTVA, Oslo, Dec. 7, 2005.

F.G. Banica

7th Polish Conference of Analytical Chemistry, Torun, Poland, June 3 - 7, 2005.

Co-author on poster presentation on: Selenomethionine as a catalyst in Ni(2+) reduction: applications to selenomethionine determination in pharmaceuticals.

XVIII International Symposium on Bioelectrochemistry and Bioenergetics, Coimbra University, Portugal, June 20 - 24, 2005.

Romanian International Conference of Chemistry and Chemical Engineering, Bucharest, Romania, Sep. 22 - 24, 2005.

Co-author on lecture on: Electrochemistry of selenomethionine in the form of a self-assembled monolayer on gold electrode surface: anodic reactions.

Research Cooperation NATO Project, at University of Pardubice, Czech Republic and Polytechnica University of Bucharest, Romania, Dec. 1 - 16, 2005.

Visit at J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic, Dec. 2, 2005. Guest Lecture on: "Electrochemical Investigations of Carotenoids in the form of self-assembled Monolayers".

Visit at University of Pardubice, Czech Republic, Dec. 6, 2005. Guest Lecture on "Prospects of Electrochemical Impedance Spectrometry for Investigation of Carbon Paste Electrodes".



D. Bedeaux

Research stay at Leiden Institute of Chemistry, Leiden, Netherlands, June 28 - July 9, 2005.

7th World Congress of Chemical Engineering, Glasgow, UK, July 10 - 14, 2005. Lecture on: "Nonequilibrium translational Effects in Evaporation and Condensation".

Conference "Thermocon 05, Messina, Italy, Sep. 25 - 30, 2005. Lecture on: "Boundary Conditions and the second Law".

L. Boman

Research Cooperation, University of Valencia, Spain, June 7 - July 2, 2005

T. Bruvoll

International Supercomputer Conference, Heidelberg, Germany, June 20 - 24, 2005.

Conference "Microsoft Tech-Ed ", Amsterdam, Netherlands, July 4 - 8, 2005.

O. Burheim

Molten Salt Discussion Group - Summer 2005, Cambridge, UK, June 14 - 15, 2005. Lecture on: "Cambridge FFC Reduction of Hematite".

PEM Summer School, Espoo, Finland, Aug. 30 - Sep. 4, 2005. Lecture on: "Measuring Contact Resistance in PEM Water Electrolysis Backing Materials".

Activities

B. Buttingsrud

The 9th Scandinavian Symposium on Chemometrics (SSC9). Reykjavik, Iceland, Aug. 21 - 25, 2005.

Poster presentation on: Superresolution of hyperspectral images.

Research stay with Professor Ross King at University of Wales, Aberystwyth, Wales, Nov. 7 - 19, 2005.

Bioinformatics Forum for Young Scientists, Randsvangen, Norway, April 15 - 17, 2005.

Lecture on: "Drug Comparison Based on Quantum Topology and Inductive Logic Programming".

P. H. Carlsen

Co-founder of new chemical company: Caliber Synthesis.

Member of PhD committees, NTNU and University of Oslo.

Member of management Committee in the EU COST D31 Program, 2 meetings in 2005, in Leuven, Belgium in March and Rome, Italy in December.

C. Chassagne

Research Stay at University of Leiden, Netherlands, Feb. 18 - March 16 and June 22 - July 25, 2005.

C. Collin-Hansen

XIII International Conference on Heavy Metals in the Environment, Rio de Janeiro, Brazil, June 5 - 9, 2005. Lecture on: "Metal Toxicity and Induction of indirect Defence Systems in the King Bolete (Boletus edulis), an edible Mushroom".

A. Fiksdahl

Board Member of the KOSK Research Program, The Research Council of Norway (2000-2006).

Deputy Head of the Board of "Faggruppen for Organisk Kjemi" (the Group of Organic Chemistry) of the Norwegian Chemical Society.

Chemistry Expert in Court on pharmaceutical Matters, Namsretten, Oslo, June 2005.

Appointed Guest Professor at Hebei University, China (2005 - 2010).

Member of International advisory Board "7th International Symposium on Biotechnology, Metal complexes and Catalysis", Beijing, China, Aug. 2005.

Mentor for female Doctoral Student, NTNU.

Conference "20. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 13 - 16, 2005.

Responsible organizer of the "Jan Bakke Seminar", NTNU, March 11, 2005.

7th International Symposium on Biotechnology, Metal Complexes and Catalysis, Beijing, China, Aug. 17 - 20, 2005. Invited Lecture on: "Synthetic Applications of Nitropyridine Derivatives".

Opponent Doctoral Thesis of Truls Ingebrigtsen, "Amines in Organic Synthesis", University of Tromsø, Norway, Sep. 23, 2005.

11th Blue Danube Symposium on Heterocyclic Chemistry, Brno, Czech Republic, Aug. 28 - Sep. 1, 2005.

A. Flatberg

Multi-way Course "Advanced Chemometric Methods", KVL, Copenhagen, Denmark, Jan. 10 - 28, 2005.

Bioinformatics Forum for Young Scientists, Randsvangen, Norway, April 15 - 17, 2005.

Lecture on: "Multiway decomposition of microarray data".

9th Scandinavian Symposium on Chemometrics (SSC9), Reykjavik, Iceland, Aug. 22 - 25, 2005. Lecture on: "Bilinear Models with Network Relations in Variables".



T.P. Flaten

Deputy Head of Department of Chemistry.

Board member, The Committee for Geomedicine of the Norwegian Academy of Science and Letters.

Editor, Norsk Epidemiologi (Norwegian Journal of Epidemiology).

Group Leader, Theme Group "Environment", The Nord-Trøndelag Health Study 3 (HUNT3).

Board member, Norwegian Chemical Society, Trondheim Branch.

Member, The Research Council of Norway, Programme Council "Drikkevannsforskning 2000" (Drinking Water Research 2000).

Meeting TEKNA/NTNU, Trondheim, Jan. 6 - 7, 2005. Lecture on: "Vannkvalitet og helse, forurensningstilførsler og drikkevannskvalitet: Kort om prosjekter fra 1. periode (1995-1999)".

Ø. Garmo

NSFTs wintermeeting; Jan. 27 - 30, 2005.
Co-author on lecture: Responses of metallothionein, superoxide dismutase and catalase in gills of Brown Trout exposed to sublethal Cd, Cu and Zn-concentrations in situ

Research stay at Lancaster University, Department of Environmental Sciences, UK, Jan. 17 - May 31, 2005.

SETAC Europe 15th Annual Meeting; May 22 - 26, 2005.

Co-author on lecture on: Responses of metallothionein, superoxide dismutase and catalase in gills of brown trout naturally exposed to sublethal Cd/Zn- and Cu-concentrations

XIII International Conference on Heavy Metals in the Environment, Rio de Janeiro, Brazil, June 5 - 9, 2005.

Lecture on: Evaluation of DGT for monitoring labile metal species in seawater.

Lecture on: "Field testing of the diffusive Gradients in thin-Films Technique for multi-Metal speciation Measurements in acid fresh Water".

Poster presentation on: Catalase and metallothionein expression and metal accumulation in differently acclimated brown trout populations exposed to a severely metal contaminated lake.

DGT Workshop 2005, Lancaster, UK, Sep. 15 - 16, 2005.

Lecture on: "Effect of Complexation on DGT Sampling of Lanthanides in multi-Metal Solutions".

O.R. Gautun

Opponent Doctoral Thesis of Anne Kristin Vibstad Bakkestuen, "Synthesis of Agelasine E and Agelasine Analogs, as well as 6-Aryl and 6-Alkenyl Purines, and Determination of their Antimycobacterial Activity", University of Oslo, Aug. 26, 2005.

K. Gellein

Society of Toxicology Annual Meeting. USA, March 5 - 10, 2005.

Co-author on poster presentation: Iron Deficient and Manganese Enhanced Diets Alter Metals and Transporters in the Developing Rat Brain.

L.H. Gidskehaug

Multi-way Course "Advanced Chemometric Methods", KVL, Copenhagen, Denmark, Jan. 10 - 28, 2005.

Bioinformatics Forum for Young Scientists, Randsvangen, Norway, April 15 - 17, 2005.

Lecture on: "Multiway decomposition of microarray data".

O. - E. Haas

IEA-AFC-PEFC & IPHE-PEFC-meeting. Mol, Belgium, June 1 - 3, 2005.

Co-author on lecture on: Development of electrocatalysts for high temperature fuel cells with polymer based electrolyte.

High Temperature PEM Fuel Cell (HT-PEM FC) Symposium Rio Patra, Greece; Sep. 13, 2005.

Lecture on: Development of gas diffusion electrodes and catalysts for PBI fuel cells at NTNU.

K. Hagen

On leave 80% of the time in order to work as elected President of the Norwegian Association of Researchers (NAR), the trade union for people in research and higher education in Norway.

Conference "11th European Symposium on Gas Electron Diffraction, Blaubeuren, Germany, June 25 - 29, 2005.

J. Holt

Conference "20. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 13 - 16, 2005.

Poster presentation on: Diazotization studies of 3-aminopyridines.

11th Blue Danube Symposium on Heterocyclic Chemistry, Brno, Czech Republic, Aug. 28 - Sep. 1, 2005.

E.E. Jacobsen

Open Day. UKA 05, NTNU, Department of Chemistry, Trondheim, Norway, Oct. 9 - 10, 2005. Artistic and museum presentation on: "Organisk kjemi på NTH før og nå". Exhibition.

M. Jartun

Meeting with the Public Road Authorities (Statens vegvesen), Oslo, Jan. 5, 2005. Lecture on: "Environmental studies at the Geological Survey of Norway".

Environmental Seminar, Harstad, Norway, March 2, 2005. Lecture on: "The Pathway from polluted Soil to polluted Sediment". A 2-hour Presentation to local, regional and national environmental Authorities.

Conference "4. Svensk-Norska Miljökemiska mötet (SNMM 2005)", Strömstad, Sweden, Sept. 4 - 7, 2005. Lecture on: "Spredning av miljøgifter fra by til havnebasseng".

National Conference "Miljøringen: Sources and Dispersion of Pollutants", Bergen, Norway, Nov. 9 - 10, 2005. Lecture on: "Dispersion of Pollutants from impervious Surfaces in Bergen".

Activities



SNBL Office. Courtesy of the SNBL

E. Johannessen

Eivind Johannessen was given the ESSO Prize for best Doctor Thesis at NTNU in 2005, in Category basic Research.

Research stay at TU Delft, Netherlands, from June 16, 2005.

ECOS 2005. Trondheim, Norway, June 20 - 22, 2005.

Poster presentation on: Diabatic tray distillation: Equipartition of entropy production as an approximation to the state of minimum entropy production.

AIChE 2005 Annual Meeting; Oct. 30 - Nov. 4, 2005. Co-author on lecture on: Optimal Porosity Distribution in Nanoporous Catalysts.

G. Kildahl-Andersen

Conference "20. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 13 - 16, 2005.

Poster presentation on: On the Carr-Price blue colour reaction of Vitamin A - First structure interpretation by NMR.

55th Meeting of Nobel Prize Winners, Lindau, Austria, June 26 - July 1, 2005.

"14th International Symposium on Carotenoids", Edinburgh, Scotland, July 17 - 22, 2005.

Lecture on: "Spectroscopic and Chemical Studies on the Carr-Price Blue Colour Reaction of Vitamin A".

Poster presentation on: Novel Diapocarotenoid Dications - Filling the Gap in the VIS-NIR Spectra of Carotenoids.

Poster presentation on: Carotenoid anions - not so easy.

Research stay at University of Alabama, Tuscaloosa, Alabama, USA, Oct. 3 - 31, 2005.

S. Kjelstrup

Advisor for Professorship in Energy Technology at KTH, Stockholm, Sweden.

Participating in two Thesis evaluation Committees at TU Delft (Peijun Ji and Lianji Xu), Netherlands.

Kjelstrup was awarded Storforsk Grant from The Research Council of Norway.

Guest Professor at Leiden University, Netherlands, June 28 - July 9, 2005.

Professor in part time Position at TU Delft, Netherlands, Oct. 1 - 14, 2005.

Organizer of the Conference "Brownian Motion one hundred Years after Einstein", Leiden, Netherlands, March 12 - 15, 2005. Lecture on: "Active Transport in slipping biological Pumps".

Organizer of "18th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, ECOS 2005", Trondheim, Norway, June 20 - 23, 2005. Lecture on: "Active Transport in slipping biological Pumps".

7th World Congress of Chemical Engineering, Glasgow, UK, July 9 - 21, 2005. Lecture on: "Heat and Mass Transfer across Phase Boundaries: Estimates of coupling Coefficients"

NordForsk Summer School: New Materials and Technologies for Low Temperature Fuel Cells, Helsinki University of Technology, Otaniemi, Finland, Aug. 30 - Sept. 2, 2005. Lectures on: "Thermodynamic Modelling of Transport Processes" and "Application of irreversible thermodynamics to polymer electrolyte fuel Cells".

NordForsk Summer School: New Materials and Technologies for Low Temperature Fuel Cells, Helsinki University of Technology, Otaniemi, Finland, Aug. 30 - Sept. 2, 2005. Lectures on: "Thermodynamic Modelling of Transport Processes" and "Application of irreversible thermodynamics to polymer electrolyte fuel Cells".

Conference "Thermocon 05", Messina, Italy, September 25 - 30, 2005. Lecture on: "Active Transport in slipping biological Pumps".

H. Koch

Research Cooperation at University of Valencia, Spain, Jan. 19 - Feb. 7, 2005.

Research Cooperation at University of Santiago de Compostela, Spain, Feb. 12 - March 1, 2005.

Research Cooperation at University of Valencia, Spain, April 16 - May 10, 2005.

Research Cooperation at University of Valencia, Spain, May 27 - July 5, 2005.

Workshop and Research Project at University of Valencia, Spain, July 15 - 31, 2005.

Conference "13th European Seminar on Computational Methods in Quantum Chemistry", Bratislava, Slovakia, Sep. 20 - 26, 2005. Lecture on: "General correlated Rotations and orbital Correlation".

Sokrates Mobility, University of Valencia, Spain, Oct. 1 - 25, 2005.

Start-up of JST Research Project, University of Nagoya, Japan, Nov. 13 - 28, 2005.

Research Cooperation at University of Valencia, Spain, Dec. 10 - 21, 2005.

T. Kumelj

Conference "ICCMSE 2005", Loutraki, Korinthos, Greece, Oct. 19 - 27, 2005.

L. Kvittingen

Research stay at Durham University, Durham, UK and University of Strathclyde, Glasgow, UK, March 14 - 18, 2005.

Preparation of a NUFU-project (Education of Chemistry Teachers for Master's Degree), University College, Dilla, Ethiopia, April 9 - 16, 2005.

3rd Int. Symp. Microscale Chem. May 19 - 22, 2005. Poster on: Enjoying enzymes

5th International Conference on History of Chemistry, Lisbon, Portugal, Sep. 6 - 10, 2005. Lecture on: "The Founding of a Chemistry Laboratory at Norway's first Institute of Technology: Laboratory Practices 1910 - 1936".

Teacher training course; "Red-Ox Chemistry-Introduction to the Portable Chemical Boxes", Stjørdal, Norway, Nov. 18, 2005.

M.I. Lian

"Det 14. seminar om hydrogeologi og miljøgeokjemi", NGU, Trondheim, Norway, Feb. 8 - 9, 2005.

Lecture on: Distribution and chemical fractionation of heavy metals in natural soils near the zinc smelter in Odda.

XIII International Conference on Heavy Metals in the Environment. Rio de Janeiro, Brasil, June 5 - 9, 2005.

Poster presentation on: Distribution and chemical fractionation of heavy metals in natural soils near a zinc smelter in Norway.

T. Ljones

30th FEBS (Federation of European Biochemical Societies) Congress and 9th IUBMB (International Union of Biochemistry and Molecular Biology) Conference, The Protein World, Budapest, Hungary, July 2 - 7, 2005.



Courtesy of the SNBL

B.F. Lutnæs

Conference "20. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 13 - 16, 2005.

Lecture on: "Delocalised Carotenoid Cations in Relation to the soliton Model".

"14th International Symposium on Carotenoids", Edinburgh, Scotland, July 17 - 22, 2005. Lecture on: "Delocalised Carotenoid Cations in Relation to the soliton Model".

2nd Borregaard Wood and Pulp Research Conference, Sarpsborg, Norway Oct. 13 - 14, 2005.

Lecture on: Analysis of lignosulphonate by NMR spectroscopy.

A. Lykknes

Interview on the Radio Programme "Verdt å vite" about Ellen Gleditch, NRK P2, June 23, 2005.

"Medisinhistorisk seminar 2005".

Lecture on: "Ellen Gleditsch (1879-1968): Professor, radiokjemiker og kvinnelig forbilde".

"Kvinnedagen", NTNU, Trondheim, Norway, March 8, 2005.

Lecture on: "Ellen Gleditsch (1879-1968): Professor, radiokjemiker og kvinnelig forbilde".

Activities

Exhibition and Lecture in NTNU's Programme on March 8, 2005. Realfagbiblioteket, UbiT, NTNU, Trondheim, Norway, March 8 - Aug. 1, 2005.

Artistic and museum presentation on: "Ellen Gleditsch - professor, radiokjemiker og kvinnelig forbilde".

Science in Scandinavia around 1905, Høgskolen i Agder, Kristiansand, Norway, May 9 - 11, 2005.

Lecture on: "Radiochemistry and the early international aspects of the career of Ellen Gleditsch (1879-1968)".

5th International Conference on History of Chemistry, Lisbon, Portugal, Sep. 6 - 10, 2005.

Lecture on: "The Founding of a Chemistry Laboratory at Norway's first Institute of Technology: Laboratory Practices 1910 - 1936".

K. Mathisen

3rd Norwegian Synchrotron User Meeting, Orkanger, Norway, March 10 - 11, 2005. Lecture on: "In-situ XAS studies on CuAPO-5 and CuZSM-5 during the selective catalytic Reduction of Nox with propane".

Research stay at the European Synchrotron Radiation Facility (ESRF) Swiss-Norwegian Beam Line, Grenoble, France, Nov. 14 - 30, 2005.

A.- K. Meland

18th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, ECOS 2005", Trondheim, Norway, June 20 - 23, 2005. Lecture on: "Rate limiting proton hydration in the hydrogen Electrode of the polymer Electrolyte Membrane Fuel Cell".

Ø. Mikkelsen

Meeting at Environment Agency, Bath, UK, Jan. 2005. Lecture on: "New Possibilities for Remote Monitoring of Heavy Metals".

Oral Hearing, European Patent Organization, Munich, Germany, Jan. 2005. Approval of the European Patent "Solid Silver Amalgam".

Meeting at Technical University, Munich, Germany, Feb. 2005. Lecture on: "Remote Monitoring of Heavy Metals".

Research stay at Equipe de Chimie Analytique et Marine de Lille, France, May 1 - Aug. 7, 2005.

Meetings at various EU/EEA Organizations, Brussels, Belgium, June 19 - 22, 2005. Lectures on: "Remote and automatic monitoring of heavy Metals".

Research work at Water Environment Monitoring Assessment and Research Center, Ministry of Water Resources, Department of Water Environment, IWHR, Beijing, China, Oct. 12 - 20, 2005.

Organizing Research Cooperation at Equipe de Chimie Analytique et Marine de Lille, Villeneuve, France, Nov. 21 - 24, 2005.

A.R. Moen

Conference "20. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 13 - 16, 2005.

Lecture on "Synthesis of both enantiomers of Ranolazine, an antianginal drug".

Poster presentation on: Synthesis of both enantiomers of Ranolazine, an anti-anginal drug.

Conference "Organisk kjemisk høstmøte", Oslo, Nov. 11, 2005.

D. G. Nicholson

Vice-Chairman of the Swiss-Norwegian Beamlines at the European Synchrotron Radiation Facility, Grenoble, France.

Board member of Norwegian Synchrotron Research AS.

Dean of Faculty of Natural Sciences and Technology until Sep. 30, 2005.

Head of Department of Chemistry from Oct. 1, 2005.

Project Cooperation at Royal Institution, London, UK, Feb. 3 - 7, 2005.

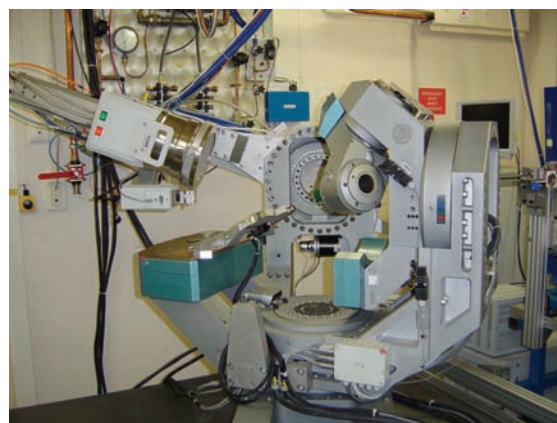
Research stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beamline, Grenoble, France, Feb. 22 - 28, 2005.

Council Meeting Swiss-Norwegian Beamline at University of Tromsø, June 7 - 10, 2005.

Research stay at the European Synchrotron Radiation Facility (ESRF), Swiss-Norwegian Beamline, Grenoble, France, June 14 - 20, 2005.

Project SNBL-ESRF, Royal Institution, London, UK, Aug. 9 - 15, 2005.

Meeting SINTEF, Oslo, Norway, Sept. 7 - 9, 2005.



Courtesy of the SNBL

C. Nordhei

Research stay at the European Synchrotron Radiation Facility (ESRF) Swiss-Norwegian Beam Line, Grenoble, France, Feb. 23 - 28, 2005.

Research stay at the European Synchrotron Radiation Facility (ESRF) Swiss-Norwegian Beam Line, Grenoble, France, Nov. 14 - 30, 2005.

V. Partali

XVIII International Symposium on Bioelectrochemistry and Bioenergetics. Coimbra, Portugal, June 19 - 24, 2005.

Poster presentation on: Electrochemistry of carotenoids in the form of self-assembled monolayer at gold surface.

14th International Symposium on Carotenoids", Edinburgh, Scotland, July 17 - 22, 2005.

Lecture on: Carotenoid amphiphiles as electron donors and triplet acceptors.

Poster presentation on: Determination of surfactant and aggregation properties of hydrophilic carotenoid derivatives.

Poster presentation on: Carotenoid thioaldehydes.

Poster presentation on: Surface and aggregation properties of the two most water-soluble carotenoids.

Poster presentation on: Facile synthesis of water dispersible carotenoids.

Poster presentation on: Stable blue carotenoids.

A. L. Ramstad

Main responsible for the Conference "3rd Norwegian User Meeting - Application of Synchrotron Radiation", in charge of the Program Group of ESRF related problems, The Research Council of Norway, Orkanger, Norway, March 10 - 11, 2005.

M.B. Rye

Multi-way Course "Advanced Chemometric Methods", KVL, Copenhagen, Denmark, Jan. 10 - 28, 2005.

Bioinformatics Forum for Young Scientists, Randsvangen, Norway, April 15 - 17, 2005.

Lecture on: "Comparing Segmentation Methods in two dimensional Gel electrophoresis".

SSC9 - 9th Scandinavian Symposium on Chemometrics. Reykjavik, Iceland, Aug. 21 - 25, 2005.

Poster presentation on: Protein spot classification by PLSR in two dimensional gel electrophoresis.

Poster presentation on: Cluster Analysis of Gene Expression Profiles Guided by Gene Ontology.

E. Ryeng

Research stay with Professor Ross King at University of Wales, Aberystwyth, Wales, Nov. 7 - 19, 2005.

Bioinformatics Forum for Young Scientists, Randsvangen, Norway, April 15 - 17, 2005.

Lecture on: "Drug Comparison Based on Quantum Topology and Inductive Logic Programming".

A. Røsjorde

18th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, ECOS 2005", Trondheim, Norway, June 20 - 23, 2005. Lecture on: "Minimising the entropy Production in a chemical Process for dehydrogenation of propane".

C. Sanz-Navarro

International Conference of Computational Methods in Science and Engineering 2005 "ICCMSE 2005", Loutraki, Korinthos, Greece, Oct. 19 - 27, 2005.

Lecture on: Molecular dynamics simulations of conformational changes in 7-helix trans-membrane receptors.

R. Schmid

11th Norwegian Seminar on Mass Spectrometry, Hafjell, Norway, Jan. 23 - 26, 2005. Lecture on: "Head-Space undersøkelser av Castoreum fra bever (Castor fiber) ved GC-MS".

K. Schrøder

Head of Department of Chemistry, until Sep. 30, 2005.

Meeting at Environment Agency, Bath, UK, Jan. 2005. Lecture on: "New Possibilities for Remote Monitoring of Heavy Metals".

Oral Hearing, European Patent Organization, Munich, Germany, Jan. 2005. Approval of the European Patent "Solid Silver Amalgam".

Meeting at Technical University, Munich, Germany, Feb. 2005. Lecture on: "Remote Monitoring of Heavy Metals".

Cooperation Project and Guest Lecture at University of Murcia, Department of Physical Chemistry, Spain, April 23 - 30, 2005. Lecture on: "Remote Monitoring of Heavy Metals".

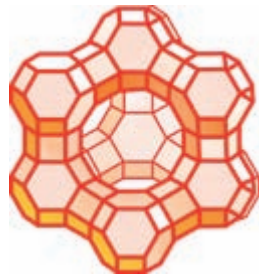
Discussions for Establishment of a Cooperation Project "Avrenning av tungmetaller fra kullgruver" with University of Copenhagen. Svalbard, Norway, June 2005.

Activities

Lecture on "Nye metoder for automatisk overvåking av tungmetaller" at Mitthögskolan/ALMI, Östersund, Sweden, June 2005. This formed the Basis of establishing a Mid-Norway / Mid-Sweden Common Project.

Meetings at various EU/EEA Organizations, Brussels, Belgium, June 19 - 22, 2005. Lectures on: "Remote and automatic monitoring of heavy Metals".

Research Stay and Profiling in USA, Battelle Research Institute, Washington DC, USA, Nov. 24 - Dec. 2, 2005. Lectures on: "Remote Monitoring of Heavy Metals".



*Zeolite
Courtesy of the SNBL*

J. - M. Simon

Diffusion fundamentals Conference 2005, Leipzig, Germany, Sep. 24 - 26, 2005. Lecture on: "Numerical Evidence for the Validity of the local Equilibrium Hypothesis: The n-octane vapor-liquid Interface".

S. Skogvold

Course "Bruk av elektrokjemisk impedans spektroskopi", University of Bath, UK, 1 week in April, 2005.

Research stay at Equipe de Chimie Analytique et Marine de Lille, France, May 2 - June 3, 2005.

Research work at Water Environment Monitoring Assessment and Research Center, Ministry of Water Resources, Department of Water Environment, IWHR, Beijing, China, Oct. 12 - 20, 2005.

Research stay at University of Bath, UK, Nov. 2 - Dec. 16, 2005.

E. Steinnes

Nordplus-seminar, Helsinki, Finland, Jan. 22 - 23, 2005.

18th Task Force Meeting of the UNECE ICP Vegetation, Almeria, Spain, Feb. 1 - 4, 2005. Lecture on: "Three Decades of Moss Surveys in Norway including 53 elements: How to interpret the data?"

"Det 14. seminar om hydrogeologi og miljøgeokjemi", NGU, Trondheim, Norway, Feb. 8 - 9, 2005.

Co-author on lecture on: Distribution of 32 trace metals in natural organic surface soils: Contribution from natural and anthropogenic sources.

8th International Conference on the Biogeochemistry of Trace Elements, Adelaide, Australia, April 3 - 7, 2005. Lecture on: "Deposition of Trace Elements from long-range Atmospheric Transport: temporal and spatial Trends in Norway".

Poster presentation on: Distribution of nitric-acid soluble fractions and organo-metallic complexes of 21 elements between different soil horizons in podzols.

1st International Workshop on Antimony in the Environment, Heidelberg, Germany, May 16 - 19, 2005. Lecture on: "Atmospheric Supply of Antimony in Norway: temporal and spatial Trends and Relations to other trace Elements".

The third International Conference on Ecological Chemistry, Chisinau, Moldova, May 20 - 21, 2005. Lecture on: "Metal Speciation in Prut River Sediments studied by Chemical Fractionation Techniques".

XIII International Conference on Heavy Metals in the Environment, Rio de Janeiro, Brazil, June 5 - 9, 2005. Lecture on: "Distribution of 32 Trace Metals in natural Surface Soils: Contributions from natural and anthropogenic Sources".

Lecture on: The use of stable lead isotopes and sequential extraction to differentiate between binding forms of natural and anthropogenic lead in Norwegian podzolic soils.

Lecture on: Long range atmospheric transport of metals: Deposition gradients in Bjørnøya, a small arctic island.

Fifth International Symposium on Modern Principles of Air Monitoring, Loen, Norway, June 12 - 16, 2005. Lecture on: "Biomonitoring of atmospheric Metal Deposition by Moss Analysis: Facts and Fallacies".

Essential Trace Elements for Plants, Animals and Humans. Reykjavik, Iceland, Aug. 15 - 17, 2005.

Co-author on lecture on: Contents of some essential trace elements in grass from cultivated meadows and vegetation from natural pastures in Western Norway: Is there an adequate supply to sheep?

Conference "4. Svensk-Norska Miljökemiska mötet (SNMM 2005)", Strömstad, Sweden, Sept. 4 - 7, 2005. Lecture on: "Fordeling av spormetaller i naturlig jord: Bidrag fra naturlige kilder og luftforurensning".

3rd Black Sea Basin Conference on Analytical Chemistry, Constanta, Romania, Sep. 12 - 14, 2005. Plenary Lecture on: "Biomonitoring of atmospheric metal deposition".

Poster presentation on: Epiphytic mosses and their substratum (tree bark) as monitors of heavy metal atmospheric deposition.

Symposium DNVA, Oslo, Oct. 13 - 14, 2005.

"Goldschmidt Lecture", NGU, Trondheim, Norway, Oct. 21, 2005.

Lecture on: "Contribution from different Sources to the elemental Composition of natural Surface Soils: What can we learn from nationwide Surveys in Norway?"

Anthropogenic Effects on the Human Environment in the Tertiary Basins in the Mediterranean. Skopje, Makedonia, Oct. 21, 2005.

Co-author on Lecture on: Biomonitoring of atmospheric metal deposition in the Republic of Macedonia.

IAEA TC Workshop on Investigation of Health Effects on Children from the Consumption of Foods grown in Industrially Contaminated Areas, Dubna, Russia, Nov. 14 - 16, 2005. Lecture on: "Nuclear methods for geomedicine".

K. Strasunskiene

Meeting on "Framtidas behov for vannkompetanse" at Telemark University College, Bø, Norway, Jan. 27, 2005.

Co-Author on poster presentation: "Kontinuerlig tungmetall overvåking i kystnært sjøvann".

F. Tjosås

Conference "20. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 13 - 16, 2005.

Poster presentation on: Pyridylmalonates; preparation and synthetic applications.

Research stay at University of Hamburg, Germany, Oct. 2005.

G. Weck

Research stay at Université Louis Pasteur, Strasbourg, France, June 20 - July 1, 2005.

Xu, Jing

Conference "Brownian Motion one hundred Years after Einstein", Leiden, Netherlands, March 12 - 15, 2005.

A. Zvolinski

11th Annual International Sustainable Development Research Conference (SDRC 2005), June 6 - 8, 2005. Lecture on: "A technology Maturity Indicator for industrial Ecology".

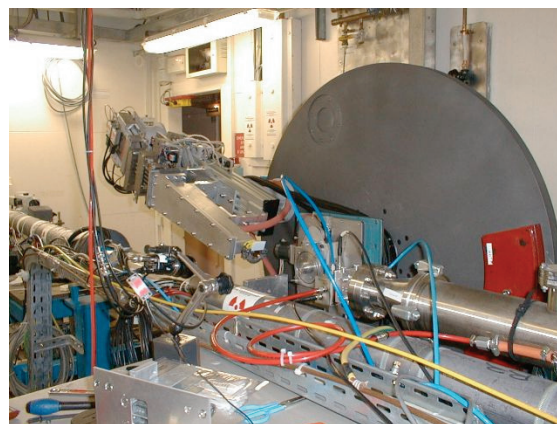
Third International Conference of International Society for Industrial Ecology (ISIE 2005); June 12 - 15, 2005.

Poster presentation on: A maturity indicator for sustainability assessment of technology in industrial ecology.

18th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, ECOS 2005", Trondheim, Norway, June 20 - 23, 2005. Lecture on: "The second Law optimal Operation of a newprint Paper drying Machine".

J.E. Aaseng

Conference "20. Organisk kjemisk vintermøte", Skeikampen, Norway, Jan. 13 - 16, 2005.



Courtesy of the SNBL

P. - O. Åstrand

Research Cooperation at University of Copenhagen, Denmark, Dec. 22, 2004 - Jan. 9, 2005.

Research Cooperation at CNRS, Grenoble, France, May 10 - 12, 2005.

Research Cooperation at University of Copenhagen, Denmark, and planning of application at Risø Research Centre, Denmark, May 17 - 20, 2005.

Conference "ICDL 2005", University of Coimbra, Portugal, June 26 - July 1, 2005.

International Conference of Computational Methods in Sciences and Engineering 2005 "ICCMSE 2005", Loutraki, Greece, Oct. 19 - 27, 2005.

Lecture on: Interaction and Equalization Models to Calculate Molecular Dipole Moments and Polarizabilities.

Paper on: Computational Molecular Science: Hybrid Classical-Quantum and Force Field.

Research Cooperation and teaching of PhD-course, University of Copenhagen, Department of Chemistry, Denmark, Nov. 28 - Dec. 9, 2005.

Spring examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/ Passed
RFEL1001	Natural Science and World Views (7,5)	Reidar Edvald Stølevik Karl Erik Zachariassen	40/33
KJ1020	Organic Chemistry (15)	Vassilia Partali	130/97
KJ2020	Organic Chemistry, Advanced Course (7,5)	Eva Henmo Mørkved	13/7
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	Helge Kjösen	14/10
KJ2024	Organic Synthesis, Laboratory (7,5)	Vassilia Partali Per Henning Carlsen	2/2
KJ2041	Physical Chemistry II (7,5)	Reidar Edvald Stølevik	2/2
KJ2043	Physical Methods in Structural Chemistry (15)	Kolbjørn Hagen Astrid Lund Ramstad Reidar Edvald Stølevik	-
KJ2050	Analytical Chemistry, Basic Course (7,5)	Knut Henning Schrøder Florinel Gabriel Banica Øyvind Mikkelsen	10/9
KJ2053	Chromatography (7,5)	Anne Fiksdahl Rudolf Schmid	14/14
KJ2070	Environmental Chemistry (15)	Eiliv Steinnes Trond Peder Flaten	19/18
KJ3055	Analytical Atomic Spectrometry (7,5)	Florinel Gabriel Banica	7/7
KJ3065	Enzyme chemistry (7,5)	Torbjørn Ljones	-
KJ8020	Advanced NMR Spectroscopy	-	-
KJ8100	Organic Medicinal and Pharamaceutical Chemistry (7,5)	Derek James Chadwick	11/10
KJ8103	Research Proposal in Organic Chemistry (7,5)	Per Henning Carlsen	-
KJ8106	Advanced Organic Chemistry (7,5)	Jan Magnus Bakke	-
KJ8200	Spectroscopy and Chemometrics (7,5)	Bjørn Kåre Alsberg	-
KJ8201	Advanced Irreversible Thermodynamics (6)	Signe Kjelstrup	1/1
KJ8202	Thermodynamics of Hydrocarbon Mixtures (7,5)	Audun Røsjorde	3/3
KJ8203	Statistical Thermodynamics and Computer Simulations (7,5)	Bjørn Hafskjold	-
KJ8204	Quantitative Structure-Activity Relationships (7,5)	Bjørn Kåre Alsberg	-
KJ8205	Molecular Modelling (7,5)	Per-Olof Åstrand	-
TKJ4105	Chromatography (7,5)	Anne Fiksdahl Rudolf Schmid	18/18
TKJ4110	Organic Chemistry, Advanced Course (7,5)	Eva Henmo Mørkved	20/16
TKJ4115	Spectroscopic Methods in Organic Chemistry (7,5)	Helge Kjösen	16/15
TKJ4130	Organic Synthesis, Laboratory (7,5)	Vassilia Partali Per Henning Carlsen	6/6
TKJ4135	Organic Synthesis, Advanced Course (7,5)	Odd Reidar Gautun	11/11
TKJ4145	Industrial Organic Chemistry, Research Projects (7,5)	Harald Rønneberg	5/5
TKJ4160	Basic Physical Chemistry and Laboratory (15)	Signe Kjelstrup Per-Olof Åstrand Henrik Koch	59/42
TKJ4165	Quantum Chemistry, Basic Course (7,5)	Henrik Koch	-
TKJ4175	Chemometrics, Basic Course (7,5)	Bjørn Kåre Alsberg	54/52
TKJ4190	Physical Chemistry, Project Work (7,5)	Terje Bruvoll	-
TKJ4195	Chemometrics, Advanced Course (7,5)	Bjørn Kåre Alsberg	-
TKJ4850	Experts in Team, Interdisciplinary Project (7,5)	-	-

Autumn examination

Course no.	Course title (credits)	Lectures and exercise coordinators	Candidates/ Passed
KJ1000	General Chemistry (15)	Thorleif Anthonen Torbjørn Ljones	187/168
KJ1030	Inorganic Chemistry (15)	Karina Mathisen	44/34
KJ1040	Physical Chemistry (15)	Reidar Edvald Stølevik Astrid Lund Ramstad	32/28
KJ2031	Inorganic Chemistry, Advanced Course (7,5)	Karina Mathisen	4/4
KJ2051	Analytical Chemistry, Advanced Course I (7,5)	Knut Henning Schrøder Florinel Gabriel Banica Øyvind Mikkelsen	9/9
KJ2090	Chemistry Education - Chemistry Dissemination (7,5)	Lise Kvittingen Per Odd Eggen	3/3
KJ2091	Teacher training/dissemination project in chemistry (7,5)	Lise Kvittingen Per Odd Eggen Knut Henning Schrøder Øyvind Mikkelsen	6/6
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)	Jan Magnus Bakke	3/3
KJ3040	Quantum Chemistry, Advanced Course (7,5)	Henrik Koch	-
KJ3056	Chemical and Sensors and Biosensors (7,5)	Florinel Gabriel Banica	8/8
KJ3058	Analytical Chemical Separation Techniques (7,5)	Rudolf Schmid	1/1
KJ3071	Applied geochemistry (7,5)	Rolf Tore Ottesen	12/12
KJ8021	Stereochemistry and Synthesis of Chiral Compounds (7,5)	Thorleif Anthonen	2/2
KJ8026	Biocatalysis in Organic Chemistry (7,5)	Thorleif Anthonen	2/2
KJ8052	Analytical Electrochemistry and its Application within Industrial and Environmental Monitoring (7,5)	Knut Henning Schrøder Øyvind Mikkelsen	6/6
KJ8070	Advanced Aquatic Chemistry (15)	Trond Peder Flaten	6/6
KJ8102	Research Proposal in Organic Chemistry (7,5)	Per Henning Carlsen	-
KJ8104	New Methods in Organic Synthesis (7,5)	Anne Fiksdahl	-
KJ8105	Organometallic Compounds in Organic Synthesis (7,5)	Odd Reidar Gautun	4/4
KJ8206	Advanced Quantum Chemical Methods (7,5)	Henrik Koch	-
KJ8207	Advanced Microarray Data Analysis (7,5)	Bjørn Kåre Alsberg	-
TKJ4100	Basic Organic Chemistry and Laboratory (15)	Per Henning Carlsen	80/66
TKJ4120	Nuclear Magnetic Resonance Spectroscopy (7,5)	Jan Magnus Bakke	13/13
TKJ4125	Natural Products Chemistry (7,5)	Elisabeth Egholm Jacobsen	11/10
TKJ4170	Quantum Chemistry, Advanced Course (7,5)	Henrik Koch	1/1
TKJ4180	Physical Organic Chemistry (7,5)	Rudolf Schmid	16/13
TKJ4185	Chemical Instrumentation and Experimental Measurements (7,5)	Terje Bruvoll	-
TKJ4200	Irreversible Thermodynamics (7,5)	Signe Kjelstrup	1/1
TKJ4205	Computational Chemistry (7,5)	Per-Olof Åstrand	2/2
TKJ4210	Inorganic Chemistry, Advanced Course (7,5)	Karina Mathisen	5/4
TKJ4700	Physical Chemistry, Specialization (22,5)	Terje Bruvoll	2/2
TKJ4725	Organic Chemistry, Specialization (22,5)	Odd Reidar Gautun	5/5

Re-sit examination

Course no.	Course title (credits)	Candidates/ Passed
RFEL1001	Natural Science and World Views (7,5)	25/22
KJ1000	General Chemistry (15)	8/5
KJ1020	Organic Chemistry (15)	17/3
KJ1040	Physical Chemistry (15)	3/1
KJ2022	Spectroscopic Methods in Organic Chemistry (7,5)	1/1
KJ2053	Chromatography (7,5)	1/1
KJ3021	Nuclear Magnetic Resonance Spectroscopy (7,5)	3/3
KJ8021	Stereochemistry and Synthesis of Chiral Compounds (7,5)	1/1
KJ8202	Thermodynamics of Hydrocarbon Mixtures (7,5)	1/1
KJ8206	Advanced Quantum Chemical Methods (7,5)	2/2
TKJ4100	Basic Organic Chemistry and Laboratory (15)	11/4
TKJ4110	Organic Chemistry, Advanced Course (7,5)	2/2
TKJ4160	Basic Physical Chemistry and Laboratory (15)	11/6
TKJ4175	Chemometrics, Basic Course (7,5)	2/1
TKJ4180	Physical Organic Chemistry (7,5)	2/1

Siv.inq. students

3. year (MTKJ)

Lervik, Anders
Høgmoen, Hanne
Melnes, Silje

4. year (SIK1)

Arstad, Ane
Berg, Michel Brunes
Eriksen, Kristine Løland
Hagen, Linda Jeanette
Haugmo, Ingvil Eide
Håland, Torfinn
Møll, Maria, Førde
Nicolaisen, Alexander
Nilsen, Robert
Reian, Gard
Vevelstad, Solrun Johanne
Vårdal, Ingeborg Herum

5. year (SIK1)

Dahl, Espen Hvidsten
Hansen, Halvor Schrøder
Jaatun, Silja
Tofteberg, Terje
Kristensen, Tor Erik Holt
Mai, Thai Trung
Mellesdal, Jardar Ingarson
Nordgård, Erland
Pettersen, Nina Marie
Stockmann, Vegar
Øpstad, Christer Lorentz

Master students

Chemistry (MKJ)

Drange, Kristine
Eggen, Ola Anfin
Frigstad, Marte Marie Hansen
Haugseth, Øyvind
Johnsen, Camilla Constance
Nordløyken, Marit
Rydningen, Marion
Sandrød, Janne
Strand, Ragnhild Beate
Tjemsland, Johanne Marie
Tronstad, Ingvild
Windju, Susanne Skrinnehaugen

Biotechnology (MBIOT5)

Midtaune, Håkon

Environmental toxicology and chemistry (MFORU)

Halkjelsvik, Anveig Bjordal

Cand.scient. students

Chemistry (MNKJ/H)

Azizyan, Mahnaz
Brustad, Håkon
Hagen, Alexander
Holm, Eva
Lindemann, Anita
Pedersen, Bjørn
Storstad, Trond Magne
Sveinhaug, Krister

Biotechnology (MNBTEK/H)

Bergene, Nina Iren
Holmgren, Kristin

PhD in Chemistry / Dr.scient. in Chemistry

PhD Einar Johan Andreassen	The use of 3-nitropyridines in synthetic organic chemistry.
Trial lecture	Synthesis and applications of quinolines and quinolones
Supervisor	Professor Jan Bakke
Evaluation committee	Professor Phil.dr. Jan Skramstad, Kjemisk institutt, Universitetet i Oslo Reader, Ph.D Thomas Gilchrist, Department of Chemistry, The University of Liverpool, England Professor Dr. ing. Anne Fiksdahl, Institutt for kjemi, NTNU
PhD Molla Mellese Endeshaw	Catalytic Enantioselective Hetero-Diels-Alder Reactions of N-Sulfinyl Dienophiles.
Trial lecture	Organocatalysis.
Supervisor	Førsteamanuensis Odd Reidar Gautun
Evaluation committee	Professor Peter Somfai, School of Chemical Science and Engineering, Royal Institute of Technology, KTH, Stockholm, Sweden Professor Lise-Lotte Gundersen, Kjemisk institutt, Universitetet i Oslo Professor Per H.J. Carlsen, Institutt for kjemi, NTNU
Dr.scient. Bente Jeanette Foss	Synthesis and Physical Properties of Hydrophilic Carotenoid Derivatives
Trial lecture	Occurrence, synthesis, modification and biological activity of flavonoids
Supervisor	Førsteamanuensis Vassilia Partali
Evaluation committee	Dr. Hansgeorg Ernst, Carotenoid Forschung, BASF AG, Ludwigshafen, Tyskland Dr. Erik Lüddecke, Carotenoid Forschung, BASF AG, Ludwigshafen, Tyskland Dr.scient. Lise Kvittingen, Institutt for kjemi, NTNU
Dr.scient. Lena Kjøbli Grønflaten	Behaviour of some nutrients and heavy metals in Scandinavian coniferous forest affected by human activity.
Trial lecture	The threat of increased mercury pollution in freshwater systems, with emphasis on changes in forestry management practices.
Supervisor	Professor Eiliv Steinnes
Evaluation committee	Dr. John Derome, The Finnish Forest Research Institute, Rovaniemi Research Station, Finland Førsteamanuensis Dr. Elin Gjengedal, Institutt for plante- og miljøfag, Norges landbrukshøgskole, Ås Førsteamanuensis Dr.ing. Trond Peder Flaten, Institutt for kjemi, NTNU
PhD Annette Lykknes	Ellen Gleditsch: Professor, Radiochemist, and Mentor.
Trial lecture	Ida Tacke Nodack - en kjemikerkarriere med for hinder.
Supervisor	Førsteamanuensis Lise Kvittingen Førsteamanuensis Anne Kristine Børresen, Institutt for historie og klassiske fag
Evaluation committee	Docent FD Anders Lundgren, Institutionen för idé- och lärdoms historia, Uppsala universitet, Sverige Professor Fil.dr. Rolf manne, Kjemisk institutt, Universitetet i Bergen Førsteamanuensis Dr.rer.nat. Vassilia Partali, Institutt for kjemi, NTNU

Post Graduate Studies

PhD Karina Mathisen

X-ray absorption spectroscopic studies on active metal sites in zeotypes during the selective catalytic reduction of NO_x with propene in an oxygen rich atomsphere

Trial lecture
Supervisor
Evaluation committee

Catalysis and the Green House Effect.
Professor David G. Nicolson
Professor Dr. Wendy R. Flavell, Department of Physics, UMITS, Manchester, UK
Overingeniør Dr. Nina Aas, Statoil Nord-Norge, Harstad
Førsteamanuensis Magnus Rønning, Institutt for kjemisk prosesseteknologi, NTNU

PhD Arne Lavrans Skuterud

Investigation of selected natural and anthropogenic radionuclides in reindeer (Rangifer tarandus tarandus) and lynx (Lynx lynx)

Trial lecture
Supervisor
Evaluation committee

Radioaktive grunnstoffer som verktøy for datering, bestemmelse av veksthastighet i planter, og transporttider i naturen.
Professor Eiliv Steinnes
Professor Knut Hove, Norges landbrukshøgskole / Norsk institutt for naturforskning
Professor Dr. Elis Holm, IKVL, Avd. för Medicinsk Strålingsfysik, Universitetssjukehuset, Lund Sverige
Førsteamanuensis Dr.scient. Tore Sivertsen, Institutt for produksjonsdyrmedisin, Norges Veterinærhøgskole, Oslo
Førsteamanuensis Dr.ing. Trond Peder Flaten, Institutt for kjemi, NTNU

Dr.scient. Karl Espen Yttri

A study of carbonaceous aerosols in the Norwegian environment, focusing on the water-soluble organic carbon fraction.

Trial lecture
Supervisor
Evaluation committee

Luftforurensning i byer - kilder, effekter og endringer over tid.
Førsteamanuensis Trond Peder Flaten
Professor Eiliv Steinnes
Avdelingsdirektør Ole Andreas Braathen, NILU
Professor Dr. Hans-Christen Hansson, Institutionen för tillämpad miljövetenskap, Enheten för atmosfärsvetenskap, Stockholms universitet, Stockholm, Sverige
Docent, Dr. Mattias Hallquist, Institutionen för kemi, atmosfärsvetenskap, Göteborgs universitet, Göteborg, Sverige
Førsteamanuensis Dr.ing. Trond Peder Flaten /
Professor Torbjørn Ljones, Institutt for kjemi, NTNU



MSc in Chemistry / Cand.scient. in Chemistry 2005

Cand.scient. Erik Fuglseth	Enantiomert rene byggesteiner fra acetovanillon
Supervisor	Professor Thorleif Anthonsen
Examiner	Professor Arne Jørgen Aasen
Cand.scient. Lars Erik Kide	Syntheses and XAS studies of anion-deficient cubic perovskites and nanosized zirconia supported copper catalysts
Supervisor	Førsteamanuensis Astrid Lund Ramstad
Examiner	Professor Leif Sæthre
MSc Gabriëlle Reijerink	Lipase catalyzed kinetic resolution for synthesis of enantiopure fine chemicals based on industrial by-products
Supervisor	Professor Thorleif Anthonsen
Examiner	Professor Arne Jørgen Aasen
MSc Tom Collin Soosainather	Syntese av enantiomert rene akrylsyreestere og bruk av disse i ringslutningsmetatose
Supervisor	Professor Thorleif Anthonsen Stipendiat Anders Riise Moen
Examiner	Professor Arne Jørgen Aasen
MSc Anne Olderdalen Steen	Studium av teknikken "Diffusive Gradients in Thin Films" for bestemmelse av frie ioner og labile spesier i sjøvann
Supervisor	Professor Eiliv Steinnes Stipendiat Øyvind Garmo Seksjonsleder Toril Inga Røe Utvik, Norsk Hydro
Examiner	Dr.scient. Bjørn Ove Berthelsen
MSc Marte Giæver Tveter	Atmosfærisk nedfall av tungmetall og PCB på Bjørnøya
Supervisor	Professor Eiliv Steinnes
Examiner	Dr.scient. Bjørn Ove Berthelsen
Cand.scient. Olav Andreas Aarstad	Undersøkelser av epimeriseringsmønsteret til mannuronan C-5 epimerasene AlgE1 og AlgE6. Karakterisering av substrat og produkt ved hjelp av spesifikke lyaser, HPAEC-PAD, ESI-MS og 1H-NMR
Supervisor	Professor Torbjørn Ljones Professor Gudmund Skjåk-Bræk
Examiner	Dr.scient. Svein Knutsen



Library

MSc in Chemistry / Siv.ing. 2005

MSc Petter Broby Aslaksen	Nucleophilic reactions of cationic vitamin A derivatives - Chemistry and spectroscopy
Supervisor	Professor Thorleif Anthonsen
Examiner	Direktør Jon Eigill Johansen
MSc Synnøve Vik Bergstad	Syntetiske studier mot (2R,3S)-N-benzoylphenylisoserin metylester, en sidekjede på taxol
Supervisor	Førsteamanuensis Odd R Gautun
Examiner	Førsteamanuensis Kåre B. Jørgensen
MSc Monica Bernhardsen	Syntese og anvendelse av polybromerte difenyletere, og Standarder for polybromerte difenyletere
Supervisor	Professor Anne Fiksdahl
Examiner	Direktør Jon Eigill Johansen
MSc Anders Endal	Triazolopyridin
Supervisor	Professor Anne Fiksdahl
Examiner	Professor Jan Skramstad
Siv.ing. Torstein Fjermestad	An ONIOM Study for Lactide Polymerization
Supervisor	Amanuensis Terje Bruvoll
	Førsteamanuensis Jon Andreas Støvneng
Examiner	Førsteamanuensis Vidar Remi Jensen
Laura Graña Suárez, International student	Nucleophilic aromatic substitution of nitropyridine
Supervisor	Professor Anne Fiksdahl
Examiner	Førsteamanuensis Kåre B. Jørgensen
MSc Jørn Hansen	Synthesis and studies of new amphiphelic compounds
Supervisor	Professor Per Carlsen
Examiner	Førsteamanuensis Kåre B. Jørgensen
MSc Eli Hiberg	Bruka av mikrofibrillert sulfitt cellulose som armering i komposittmaterialer
Supervisor	Professor Anne Fiksdahl
Examiner	Professor emeritus Torbjørn Helle
Siv.ing. Kjersti Ruud	Kjemoenzymatisk syntese av enantiomert rene sekundære alkoholer fra α,β-umettete karboksylsyrer
Supervisor	Professor Thorleif Anthonsen
Examiner	Professor Arne Jørgen Aasen

The following Dr.ing./Ph.D. projects are in progress:

Student	Title	Thesis advisor
Andreassen, Trygve PhD	Asymetriske ene-reaksjoner med aza-analoger til svoveldioksid.	Odd Reidar Gautun
Boman, Mats Henrik Linus PhD	Analytical coupled-cluster calculation of gauge invariant optical properties.	Henrik Koch
Burheim, Odne Stokke PhD	Elektronisk utfelling av jern. (eng.: Electrowinning of iron from chloride melts).	Signe Kjelstrup
Buttingsrud, Bård PhD	En forbedret metode for sammenlikning av 3D Molekylelektronstrukturen i rasjonell legemiddeldesign.	Bjørn Kåre Alsberg
Flatberg, Arnar PhD	Simulation of microarray experiments and protosomic 2D gel electrophoresis.	Bjørn K. Alsberg
Garmo, Øyvind Aaberg PhD	DGT – a new assessment tool for toxic metals in Norwegian Aquaculture.	Eiliv Steinnes
Gellein, Kristin PhD	Trace elements and health – in vitro, experimental animal and human population studies.	Trond Peder Flaten
Gidskehaug, Lars H. Dr.ing.	Chemometric methods for variable-selection and normalisation of microarray-data.	Bjørn K. Alsberg
Glavatskiy, Kirill Sergeevich PhD	Multi-component evaporation as described using the Nonequilibrium van der Waals square gradient model.	Dick Bedeaux
Gonzales, Susana Villa PhD	Synthesis of optically active surfactants and the study of their properties.	Per Carlsen
Holt, Jarle PhD	Nitropyridyl isocyanate.	Anne Fiksdahl
Haas, Ole-Erich PhD	Transport on a nanoscale; at surfaces and contact lines in PEM fuel cells.	Astrid Lund Ramstad
Kildahl-Andersen, Geir PhD	Chemoenzymatic Methodes for Synthesis of Rnantiopure Biologically Active Compounds. (Kjemoenzymatiske metoder for syntese av enantiomert rene biologisk aktive stoffer).	Thorleif Anthonsen
Kumelj, Tjasa PhD	Free energy calculations of ligand-protein interactions.	Per-Olof Åstrand
Meland, Anne-Kristine PhD	Optimalization of Pemfc Anode Reaction.	Signe Kjelstrup
Moen, Anders Riise PhD	Synthesis of enantiopure fine chemicals and drugs	Thorleif Anthonsen
Nordhei, Camilla PhD	Structural Studies of Functional Oxides and their Catalytic Behaviour –XAS and XRD Studies of Nanophase Spinels.	Astrid Lund Ramstad
Rye, Morten Beck PhD	Scale space based image registration of proteomic gels.	Bjørn K. Alsberg
Ryeng, Einar PhD	Analyse av mikromatrisedata med induktiv logikk-programmering.	Bjørn K. Alsberg
Skogvold, Silje Marie PhD	Overvoltage in Voltammetry: Fundamental Processes, related to Analytical Sensor Development for Online and Remote Trace Analyses.	Knut Schrøder

Post Graduate Studies

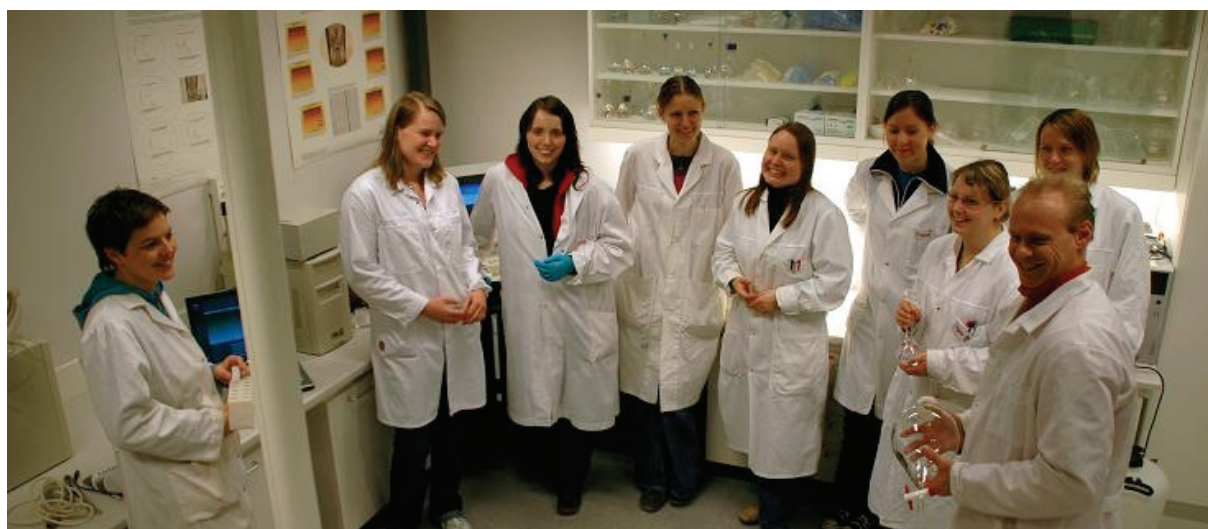
Strasunskiene, Kristina	PhD	Automatically measuring systems for heavy metals and trace Metals in waste water from sewage discharge and incineration plants. Early warning systems.	Knut Schrøder
Tjosås, Freddy	PhD	Fused heterocycles from nitropyridines.	Anne Fiksdahl
Xu, Jing	PhD	A Nonequilibrium Molecular Dynamics Simulation Study of Chemical Reactors	Signe Kjelstrup
Yu, Qiang	PhD	Synthesis of Nucleic Base containing oligomers and polymers.	Per H. Carlsen
Zvolinschi, Anita	Dr.ing.	On exergy analysis and entropy production minimization in industrial ecology.	Signe Kjelstrup
Aaseng, Jon Erik	PhD	Asymmetric synthesis of substituted 2-aminotetralins. (Asymetrisk syntese av substituerte 2-aminotetraliner).	Odd Reidar Gautun

External students

Student	Title	Thesis advisor	
Hokstad, Jorunn Nerbø	Dr. ing.	Interactions between oil, surface-active agents and water: An organic analytical study of processes taking place when marine oil spills are treated with oil spill agents.	Anne Fiksdahl
Ingebrigtsen, Stian	PhD	Elektroniske prosesser i flytende dielektrika under høye eektriske feltpåkjenninger.	Per-Olof Åstrand
Jartun, Morten	PhD	Urban risk – Dispersion mechanism and possible health effects of PCB in the urban environment.	Eiliv Steinnes
Karstensen, Kåre Helge	Dr.scient.	Miljøeffekter i sementproduksjn knyttet til klor i brensel og råmaterialer.	Eiliv Steines
Li, He	PhD	Modifikasjon av carotenoider (eng.: Modification of carotenoids).	Vassilia Partali
Lian, Monica Ihlebæk	PhD	Systemanalyse av metallforurensning i det terrestriske miljø i Odda-området.	Eiliv Steinnes
Løkken, Torbjørn Vegard	PhD	Analyser av vandduggpunkt og hydrokarabonduggpunkt i naturgass. (eng.: Determination of water dewpoint and hydrocarbon dewpoint in natural gas).	Rudolf Schmid
Størseth, Trond Røvik	PhD	Crysolaminarans from marine diatoms: Structural characterization and potential as immunostimulants.	Vassilia Partali
Sørbye, Karsten Alstad	Dr. ing.	Dihydroksyacetonderivater, fremstilling og reaktivitet.	Per Carlsen
Aarhaug, Thor Anders	PhD	Ny membrane for polymer brenselsceller.	Signe Kjelstrup

Student exchange from NTNU, Department of Chemistry 2005

Name	Specialization	Level	Institution
Hans Eirik Stuenes Haarberg	Biochem.	BSc, 3th yr	Iowa State University, USA
Halvor Schröder Hansen	Phys.chem.	MSc, 4th yr	ETH Zürich, Switzerland
Cheau Ling Poon	Phys.chem.	MSc, 4th yr	University of Auckland, Australia
Terje Tofteberg	Phys.chem.	MSc, 4th yr	TU Berlin, Germany
Marte Marie Hansen Frigstad	Org.chem.	MSc, 4th yr	Institute for Chemical and Environmental Research, Barcelona, Spain
Tor Erik Kristiansen	Org.chem.	MSc, 5th yr	University of Hawaii, Manoa, USA
Vegar Stockmann	Org.chem.	MSc, 5th yr	University of Hawaii, Manoa, USA



Students in the laboratory with Øyvind Mikkelsen

Student exchange to NTNU, Department of Chemistry 2005

Cayuela, Iris	Universidad de Almeria, Spain
Guziejewski, Dariusz	University of Lodz, Poland
Kunova, Kathrin	Universität Hamburg, Germany
Leifert, Annika	RWTH, Aachen, Germany
Maier, Britta	RWTH, Aachen, Germany
Raiber, Tim	Universität Hamburg, Germany
Sielk, Jan	RWTH, Aachen, Germany
Stern, Daniel	Georg-August-Universität, Göttingen, Germany

Scientific staff



Professor, Dr.scient.
Bjørn Alsberg



Assistant Professor
Terje Bruvoll



Associate Professor, Dr.ing.
Trond Peder Flaten



Professor, Dr.ing.
Thorleif Anthonen



Professor, Ph.D.
Per Carlsen



Associate Professor, Dr.ing.
Odd Reidar Gautun



Associate Professor, Dr.ing.
Florinell Banica



Adjunct Professor, Ph.D.
Derek Chadwick



Professor, Dr.philos.
Kolbjørn Hagen



Adjunct Professor, Dr.philos.
Dick Bedeaux



Professor, Dr.ing.
Anne Fiksdahl



Dr. Scient
Elisabeth Egholm Jacobsen



Professor, Dr.techn.
Signe Kjelstrup



Ph.D.
Karina Mathisen



Associate Professor, Dr.scient.
Astrid Lund Ramstad



Professor, Ph.D.
Henrik Koch



Professor, Ph.D.
David Nicholson



Associate Professor, Dr.rer.nat.
Rudolf Schmid



Associate Professor, Dr.scient.
Lise Kvittingen



Adjunct Professor
Rolf Tore Ottesen



Professor, Dr.philos.
Knut Schrøder



Professor, Ph.D.
Torbjørn Ljones



Associate Professor, Dr. rer.nat.
Vassilia Partali



Professor, Dr.philos.
Eiliv Steinnes

Staff



Professor, Dr.philos. Reidar Stølevik



Professor, Ph.D. Per-Olof Åstrand

Professor emeritus, Dr.techn.
Jan Bakke

Professor, Dr.techn.
Bjørn Hafskjold
(Leave of absence)

Professor emeritus, Dr.techn.
Synnøve Liaaen Jensen

Associate professor, Dr.techn.
Helge Kjøsen,
to July 31st, 2005

Associate Professor, Dr.ing.
Eva Mørkved,
to October 31st, 2005

Professor emeritus, Dr.philos.
Marit Trættemberg

Administrative staff



Head of administration
Anne Langseth



Senior consultant
Lillian Hanssen



First secretary
Aase Sæther



First secretary
Inger Marie Frøseth



Consultant
Ingrid Kristine Tømmerdal

Technical staff



Senior Engineer
Stein Almo



Chief Engineer
Syverin Lierhagen



Technician
Gunnar Svare



Senior Technician
Julie Jackson



Technician
Kjersti Ljones



Engineer
Kari Tanem



Technician
Nina Klausen



Chief Technician
Tron Rolfsen



Technician
Roger Aarvik

Scientific Assistants

Andreassen, Trygve
Boman, Linus
Buttingsrud, Bård
Endeshaw, Molla Mellese
Flatberg, Arnar
Gidskehaug, Lars Halvor
Gonzalez, Susana Villa
Haas, Ole-Erich
Hårklau, Halvard
Jacobsen, Elisabeth Egholm
Jartun, Morten
Karstad, Rasmus
Kildahl-Andersen, Geir
Kvidal, Marit
Midtaune, Håkon
Mikkelsen, Øyvind
Moen, Anders Riise
Nordhei, Camilla
Rye, Morten Beck
Skogvold, Silje Marie
Storstad, Trond Magne
Strasunskiene, Kristina
Størseth, Trond Røvik
Tjosås, Freddy
Tronstad, Ingvild
Zvolinschi, Anita
Øvergård, Tommy
Aaseng, Jon Erik

Undergraduate Assistants

Abrahamsen, Iren
Alsvik, Inger Lise
Bolstad, Kjersti Hysing
Dahl, Espen Hvidsten
Drange, Kristine
Eggen, Ola A.
Ellingsen, Christian
Fahadi, Jalal
Frafjord, Anders Malm
Frigstad, Marte
Fugleneb, Astrid Kobro
Gundersen, Tony Håland
Haas, Ole-Erich
Hermann, Solveig
Høgetveit, Sigrun Ø.
Høien, Are Håvard
Håland, Torfinn
Haarberg, Hans Eirik
Karstad, Rasmus
Lian, Nikolai
Lystvet, Sina Maria
Melnes, Silje
Midtaune, Håkon
Nordgård, Erlend
Nordløyken, Marit
Noreng, Lars Erik
Poon, Cheau Ling
Reijerink, Gabrielle
Schei, Jørgen
Skårn, Jenny Skeide
Soosainather, Tom Colin
Stormoen, Ragnhild B.
Storstad, Trond Magne
Vestrum, Ragnhild Inderberg
Vevelstad, Solrun Johanne
Wist, Turid
Øpstad, Christer L.

Guest professors/researchers/lecturers

Svetlana Demkina,	Jan. 15 - April 15, 2005
Carmen Donisa,	Feb. 9 - 28, 2005
Miguel Rubi,	Feb. 15 - March 3, 2005
Marina Frontasyeva,	March 8 - 19, 2005
Pieter Schmal,	from May 23 - June 25, 2005
Ana Ion, Aug.	11 - Sept. 30, 2005
Jean-Marc Simon,	from Aug. 1, 2005
Gregor Luthe,	to Dec. 31, 2005
PhD Student Gary Urb,	Oct. 10 - 31, 2005
PhD Student Anjan Patel,	to March 30, 2005
IASTE Student Jiong Zou,	Sep. 28 - Dec. 31, 2005
Madame Curie Student Sten Richard Sott,	from Oct. 1, 2005

Professor Curt Wentrup, University of Queensland, Australia Sep. 7, 2005:
Student orientation meeting. "Opportunities for Study Abroad at the University of Queensland".

Professor Curt Wentrup, University of Queensland, Australia Sep. 9, 2005:
"Chemistry of Iminopropadienones, R-N=C=C=C=O".

Dr. Finn Achmann, Aalborg University, Denmark Sep. 29, 2005:
"How can Nuclear Magnetic Resonance (NMR) be Applied to Characterize the Inclusion Complexes between Cyclodextrins and their Guest Molecules".



Annual Report for Department of Chemistry, NTNU

NTNU – Innovation and Creativity

The Norwegian University of Science and Technology (NTNU) in Trondheim represents academic eminence in technology and the natural sciences as well as in other academic disciplines ranging from the social sciences, the arts, medicine, architecture to fine arts. Cross-disciplinary cooperation results in ideas no one else has thought of, and creative solutions that change our daily lives.

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