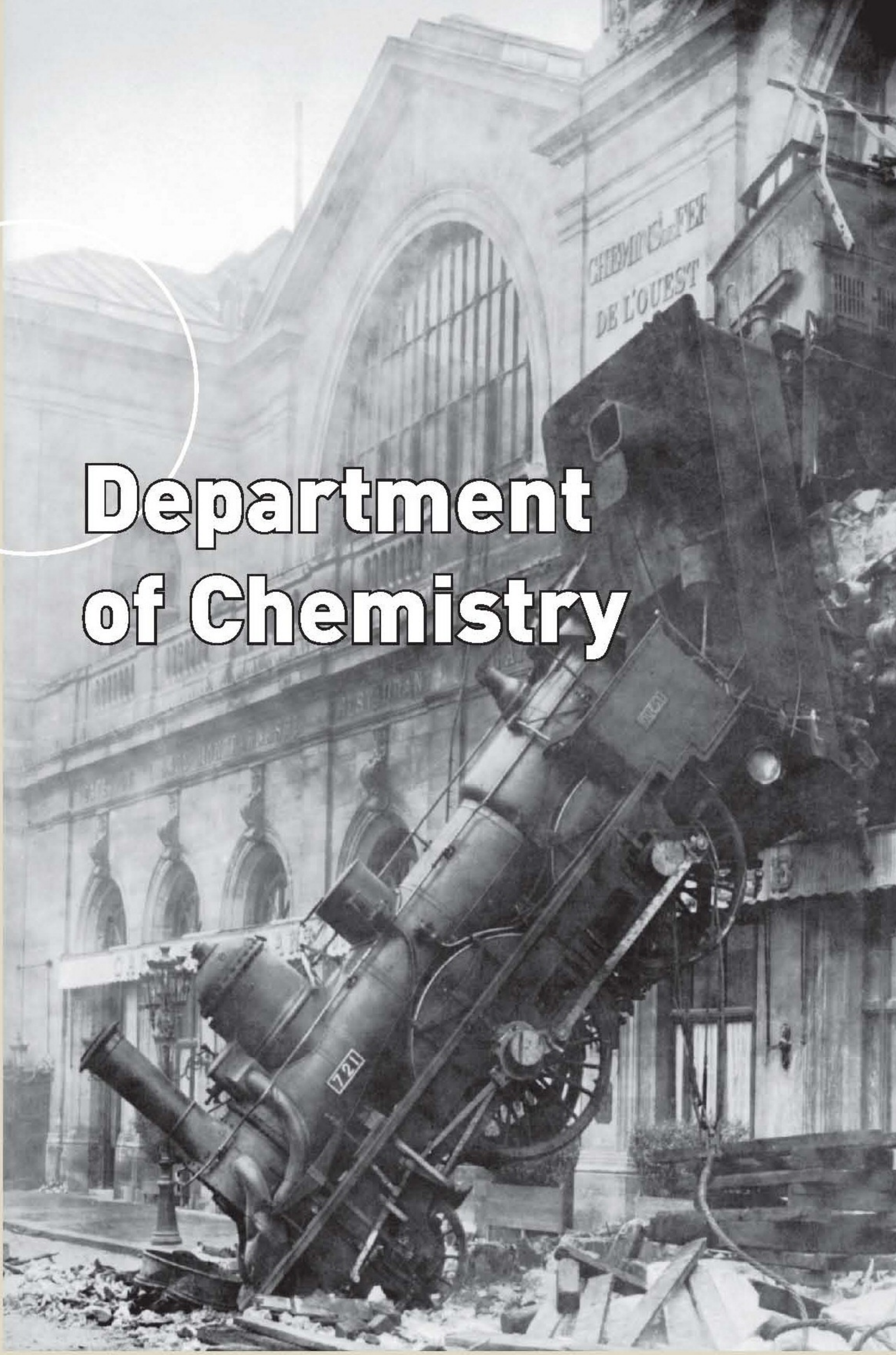
# Department of Chemistry

# Annual Report 2007



NTNU
Innovation and Creativity

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**COVER PAGE**

"A metaphor for inadequate investment in the university sector."

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# The State of the Department of Chemistry 2007

Paradoxically these are turbulent times for university funding despite a booming national economy. Yet again cut-backs have had a deleterious effect on the Department´s finances in 2007 with no respite being likely next year. A comparison between us and Chemistry at the University of Bergen is not to our advantage; although the departments are of similar size the latter receives a 20% larger grant.

The process of restructuring the scientific profile of the Department that was initiated in 2006 was carried over to 2007 by our Strategy Seminar at Jægtvolden. The process took into consideration the vision of the University Governing Board that NTNU will be the highest ranked Norwegian university and amongst the ten best in Europe within 2020. The question was raised: is this commendable goal actually achievable for a university operating in an increasingly restrictive economic climate? Under the current situation this ambition is simply not commensurate with current economics and indeed creates considerable irritation amongst the staff.

**Cutbacks**

Of course although our response to the economic realities must be to cut back on costs we are doing our utmost to maximise support to research. In this regard we are particularly cognisant of our commitments to our PhD students. Therefore, economic necessity led to seven courses being cancelled over the past few years. An important factor is to achieve an overall 50:50 split between teaching load and research. In particularly, cost-cutting has impacted negatively on the implementation of the Government´s Quality Reform in Higher Education – but then, sufficient funds supporting this have not been forthcoming. We have also implemented measures to stimulate those activities that generate external income whilst balancing this against the requirement that the Department carries out quality basic research. The effects of such initiatives take time before they bear fruit.

*Figure: Everything is being done to maximise the Departments activities.*

**Opportunities and production**
Nevertheless, the past year has also been one of opportunities and we have published 65 papers in international journals. Other activities include:

- Working with StatoilHydro on an ambitious project that includes a Canadian university. The subject of the project is connected to the company's shale oil interests.

- An International Masters Degree course involving StatoilHydro, SINTEF and others with the focus being environmental chemistry of polar regions.

- Secondment of Professor Signe Kjelstrup to the Centre of Advanced Studies in Oslo as Head of the Chemical Process Design Group

- Started organising The Nordic Synchrotron Radiation Initiative Kick-off Meeting to be held at Jægtvolden Fjord Hotel in April 2008.

- The Department has a proactive approach to recruiting women. We have an initiative in place for identifying and encouraging external female applicants to apply for vacant academic positions.

- A project financed by the 7th Framework Programme of the European Union, DeCarbit. This is a collaboration between Air Liquid France, SINTEF, the Department of Chemistry and ten other partners throughout Europe.

- Forum for Research Collaboration between the Faculty´s departments.

- Action Plan from the Jægtvolden Stategy Seminar

- The number of student applicants to the BSc programme was reduced from 40 to 30 in order to focus on the better qualified students.

- The Department produced 19 MSc and 7 PhDs.

- Three promising areas for innovation were carried over from the previous year. NTNU´s Technology Transfer Office (TTO) is integral to this process.

**Strategic Plan - Implementation**
Appointing new members of the academic staff is the most strategic long-term implementation of the Strategic Plan. An important question concerning the level of staffing is: What should the size of the Department be? The overriding factor that defines this is teaching. Positions falling vacant are subjected to critical review and, since teaching is research-based and we aim for a 1:1 teaching:research ratio, it is the teaching load borne by the Department as a whole that dimensions the Department. However, economic realities force us to balance this against the fact that over 90% of the Department´s grant from NTNU is already consumed by salaries. For this reason, the Department has not (yet) been fully compensated for the shortfall as staff retire. Nevertheless, in 2007 we did appoint three new associate professors: Annette Lykknes, Chemical Education; Morten Bjørgen, Physical Chemistry and Nebosja Simic, Organic Chemistry.

There are currently eight women amongst the 30 academic staff and two female Emeritus Professors.

We congratulate two of our female staff (Lise Kvittingen and Vassilia Partali) on their promotions to full professor.

As always, the Head´s job is made easier by dedicated staff and collaborative colleagues, and I am grateful to all those who have assisted me.

*David G. Nicholson*
*Head of Department*

# The PryJector: A device to make the invisible visible

In many situations there is an interest in knowing the spatial distributions of compounds and properties. Typical example applications can be found in the medical, forensic and military fields. For example, locating the presence of blood on surfaces in crime scene analyses or the detection of explosive residues in anti-terrorism work.

The most effective way to extract chemical information from a surface without using wet-chemical analyses, is to employ spectroscopy. Of particular interest is the use of vibrational spectroscopies such as Raman, near and mid-infrared although UV and X-ray spectroscopies are also possible. Light interacts with matter to generate chemical (and physical) signals that contain information. It is often the case that extracting this information is so complex that advanced data analytical techniques are necessary. Various methods for this task are available within the field of chemometrics. These perform by a process of "unmixing" from which the concentrations and spectral profiles of individual mixed components can be inferred. In most realistic situations this is necessary because mixtures cannot be assumed to contain a single wavelength selectivity for the compounds of interest.

So how can spectroscopy be applied to whole surfaces? The answer is to combine imaging and spectroscopy into one single instrument – a so-called **hyperspectral camera**. This is a technology which originates from the field of remote sensing and is increasingly being applied to many other areas such as medicine, the food industry and specific areas of chemistry.

The result from a hyperspectral camera is a stack of grey scale images, one for each wavelength. This "hypercube" of data can then be analysed with e.g. chemometric methods to extract the chemical information that is contained in each pixel. The result is a **chemical image** which looks like an ordinary image except that the intensity of every pixel is related to e.g. the concentration or presence (absence) of a particular chemical compound (or property). Consequently, the chemical image identifies locations in the original scene where the chemical information of interest is present.

The PryJector device is basically a modified hyperspectral camera with an image projector. The projector may be an ordinary colour computer projector or a laser. The PryJector takes the chemical image and projects it **back onto the surface** which was analysed. This means the PryJector makes the chemical information available *in situ* which is an advantage in situations where inspection of the results on a computer monitor is not optimal. Two applications are given to illustrate this:

- **Surgery**. The surgeon is in need of information about the chemical and biological state of tissue surfaces. Averting his eyes to a monitor is possible, however current modern operating theatres are already close to overloading medical staff with information. In addition, when several surgeons and nurses need to rapidly access the same information obtained from a hyperspectral instrument, the use of ordinary computer monitors can be a hindrance.
- **Crime scene investigation**. Forensic experts inspecting a crime scene need to access a wide range of chemical compounds and biological material on complex surfaces. Manual inspection is important and the use of a portable computer monitor is impractical in many situations. If the processed results from a hyperspectral camera are available as projected false coloured spots on surfaces, it will facilitate the process of localising potentially useful evidence material.

A patent application for the PryJector has been submitted via our Technology Transfer Office (TTO) at NTNU. However, projection is not the only part of the invention. There is also described a solution which enables the hyperspectral camera to process chemical images almost in real time. The reason for this is that in order for the PryJector to be useful in field work where the scene under study is changing rapidly, the current slow hyperspectral technology cannot be used. The invention therefore includes a proposal for speeding up the process by connecting the prediction of chemical images together with the scanning process. This means that the very large "hypercube" is never stored, something which will reduce scanning time significantly.

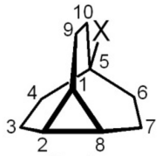
*Bjørn K. Alsberg*

# Cage hydrocarbons. The molecular structure of tricyclo[3.3.2.$0^{2.8}$]decane (Hexahydrobullvalene; 3b) – A Gas-Phase Electron Diffraction (GED) Study

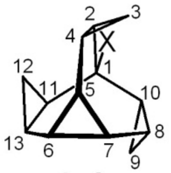
In relation to unbridged tertiary carbocations, bridgehead carbenium ions in bicyclic and higher oligocyclic systems are generally destabilised, since a severely increasing angle strain prevents them from adopting the preferred trigonal planar configuration. As has been demonstrated earlier, the bridgehead cations with a bicyclo[2.2.2]octyl and a tricyclo[3.3.2.$0^{2.8}$]decyl (hexahydrobullvalenyl) skeleton are stabilised significantly, when three cyclopropyl groups are annelated across the two-carbon bridges adjacent to the bridgehead carbenium ion centre. In absolute terms, the solvolysis rate of the bridgehead chloride of trishomobullvalene **4b** is 3070 times as high as that of 1-chlorotrishomo¬bar¬relene **2b**. Yet the rate due to the three α-cyclopropyl groups in 1-chlorotrishomobullvalene **4b** relative to 5-chlorotricyclo-[3.3.2.$0^{2,8}$]decane (**3b**) is only enhanced by a factor of 3.9x$10^6$, whereas the rate ratio is 2.8x$10^8$ for 1-chlorotrishomobarrelene **2b** relative to 1-chloro-bicyclo[2.2.2]octane (**1b**).

**1a**,**b**

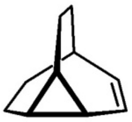
**2a**,**b**



**3a**,**b**



**4a**,**b**



**5**

**a** X = H
**b** X = Cl

This difference in the rate ratios correlates very well with the difference in the torsional angles between the planes of the α-cyclopropyl groups and the axes of the empty bridgehead orbitals in the cationic intermediates, and the absolute difference in solvolysis rates of **4b** and **2b** relates to the flattened bridgehead in the skeleton **4a**. Such a flattening along with a greater flexibility should also be observed for the inner skeleton of **4a**, the hexahydrobullvalene **3a**. In order to rigorously prove this hypothesis, we tried to determine the bridgehead bond angles in tetrahydrobullvalene, **3a**, by X-ray crystallography and by gas-phase electron diffraction.

Attempted crystal structure determinations failed, probably because the **3a** molecules have a nearly spherical shape and form plastic phases in which the molecules are orientationally disordered, thus a gas-phase electron diffraction study is the method of choice for determining the structural parameters of **3a**.

The molecular structure of tricyclo[3.3.2.$0^{2.8}$]-decane (hexahydrobullvalene) has been determined experimentally by gas-phase electron diffraction as well as by quantum chemical calculations. The bond lengths in the skeleton [1.496(7) in the cyclopropane ring, 1.527(10) adjacent to it, 1.550(22) for the central bonds in the bridges and 1.548(16) Å for the bonds originating from the singular bridgehead all can be explained in terms of the features of this cage hydrocarbon. All three C,C,C-valence angles [113.0(8)° at the singular bridgehead, 112.8(12)° adjacent to it and 122.3(20)° adjacent to the skeletal cyclopropane ring] are larger than the regular tetrahedral angle on an $sp^3$-hybridized carbon atom. The two-carbon bridges between the skeletal cyclopropane ring and the opposite bridgehead are twisted with a dihedral angle of 43°, i. e. significantly smaller than the 60° in *n*-butane in its *synclinal (gauche)* conformation.

At first glance it may appear puzzling that the cyclopropyl C-C bond in **3a** (1.496 Å) is found to be somewhat shorter than in cyclopropane itself (1.542 Å) [5] and in trishomobullvalene (**4a**) (1.542 Å) [4]. On second thoughts, however, the difference in this bond length for 3a on one side and bullvalene as well as **4a** on the other can be rationalised as being a consequence of the larger bonding angles of 126.3° and 123.8° on the ethylene and cyclopropane bridges, respectively, in the latter two cage hydrocarbons, which must exert a stretching effect on the bonds in the skeletal three-membered ring.

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*Marit Trætteberg*

# Making gasoline from coal or natural gas: Hints to rational catalyst design from fundamental mechanistic insights

**Methanol to hydrocarbons -MTH**

The current high oil prices have sparked interests in technologies that utilize natural gas, coal or even biomass rather than liquid petroleum for production of transportation fuels and raw materials for the petrochemical industry.

Methanol, which may be manufactured from any gasifiable carbonaceous material constitutes a convenient intermediate in this respect, because it can be converted into gasoline and polymer grade alkenes over solid acidic catalysts.

The breakthrough in MTH chemistry came by the pioneering work in the seventies by researchers at Mobil who (accidentally!) discovered that methanol is converted with high efficiency into gasoline over their new zeolite ZSM-5. Later, processes designed for gasoline- and alkene production from methanol have been demonstrated on pilot- and industrial scale.

**The MTH catalyst: Zeolites**

The MTH reaction is zeolite facilitated. Zeolites are naturally occuring, highly porous crystalline aluminosilicates with sharply defined channels and pores of molecular dimensions (Figure1).

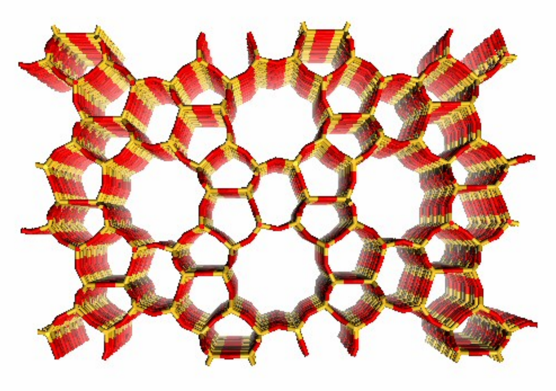

*Figure 1. The ZSM-5 (MFI) zeolite*

Zeolite frameworks are overall anionic, and charge compensating protons are located in the nano pores to maintain overall electrical neutrality. Thus, protonated zeolites are solid Brønsted acids, and their acidic strength is in line with that of 80 % sulfuric acid. The importance of zeolites in chemical industries can hardly be overestimated and in the petroleum refining industry, catalytic cracking is by far the largest application, followed by hydrocracking.

**How can possibly two or more methanol molecules combine and form alkenes by the aid of a zeolite?**

Despite of more than 20 mechanism proposals, the answer to this question is most likely that they can't. So far, no studies have evidenced that methanol molecules can be coupled directly into hydrocarbons at rates significant for the steady state operating catalyst. An indirect reaction route, known as "the hydrocarbon pool mechanism", was conceptually introduced in the early 1990s and has gradually been generally accepted. The hydrocarbon pool can be described as a catalytic scaffold, constituted by larger organic molecules (adsorbed in the working zeolite) to which methanol is added, and alkenes are eliminated from in a closed catalytic cycle. The hydrocarbon pool species identified up to now have been hexamethylbenzene (or its protonated counterpart) and the heptamethylbenzenium cation. Both these species are able to split off light alkenes under formation of the corresponding lower polymethylbenzene homologue. The lower polymethylbenzene is then methylated by methanol repeatedly until the higher active species has been formed and the catalytic cycle has been closed.

**The specifics of the MTH reaction mechanism over zeolite H-ZSM-5.**

Quite early in our research on H-ZSM-5, the experiments showed that the previously suggested hydrocarbon pool mechanism could not be valid for this catalyst. Hexamethylbenzene were certainly present in copious amounts in H-ZSM-5 during the MTH reaction, but in stark contrast to all previous conclusions, hexamethylbenzene turned out to be virtually inert when confined in the ZSM-5 channels. As a direct implication of this, a hydrocarbon pool mechanism involving hexamethylbenzene, proven to be all dominating for other zeolites, cannot be applicable for H-ZSM-5. Rather, we found that

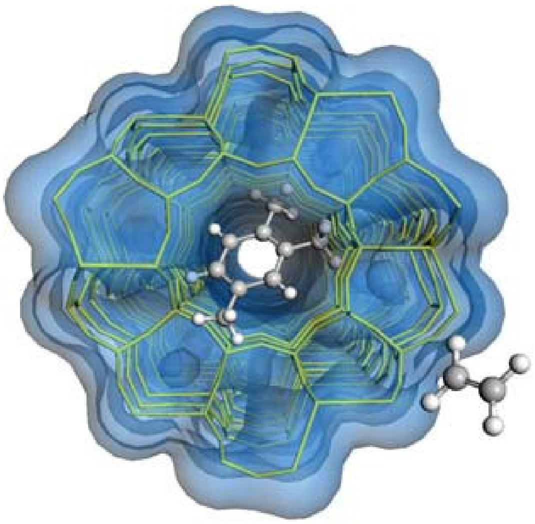

*Figure 2. The active confined species in H-ZSM-5 produces ethene from methanol*

ethene is formed exclusively from the trimethylbenzenes whereas propene and higher alkenes are mainly formed from an additional cycle involving alkene methylations and – interconversions. These two statements, implying that the ethene formation is mechanistically separated from the formation of propene and higher alkenes, are of utmost importance for understanding and possibly controlling the ethene/propene selectivity in MTH catalysis. Our findings lead to an interesting question both regarding mechanistic understanding and selectivity control: Do the cycle for ethene formation run completely independently of the cycle for higher alkene formation? We believe that this is not the case, as the higher alkenes continuously form new aromatic species. On the contrary, the cycle for ethene formation is probably not required for the higher alkene cycle to run.

So in in conclusion, if it is possible to completely separate the two cycles by sterically supressing the formation of the larger aromatics, formation of the undersired ethene might be avoided in an industrial methanol-to-propene (MTP) application.

*Figure 3. The selectivity aspects of the MTH reaction revealed the last few years are relevant for upgrading of natural gas.*

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*Morten Bjørgen*

# Quasi-Elastic Neutron Scattering Investigation: Diffusion of Hydrogen in Carbon Materials.

This is a PhD program in structural physical chemistry, and a part of the “Storforsk” project entitled “Transport on a nanoscale; at surfaces and contact lines in PEM fuel cells” led by Signe Kjelstrup with Astrid Lund Ramstad as PhD supervisor. The project includes theoretical and experimental work. In this PhD program we focus on the diffusion of hydrogen in the carbon material that is used in the PEM fuel cell.

**Our first neutron experiment**
In this work, we are studying the interactions between the surface of Vulcan XC-72R, an amorphous carbon and the hydrogen molecules that pass through the graphite matrix. The aim is to find the diffusion coefficient of hydrogen molecules on the surface of this material. This is fundamental to understanding the PEM fuel cell, and the transport phenomena of reactants to the catalyst particles.

In November 2006 we performed our first quasi-elastic neutron scattering experiment by using the Time-of-flight (TOF) spectrometer IN5 at the Institute Laue-Langevin (ILL) in Grenoble. The TOF spectrometer measures the velocity of neutrons before and after interaction with our carbon and hydrogen sample, thereby providing information on the exchange of energy and momentum between atoms and neutrons. In turn, this gives information about the different types of energy barriers that the atoms inside the samples must overcome, and how they are moving. Neutron spectrometry was chosen to investigate hydrogen diffusion because the characteristics of hydrogen in a neutron beam make it easy to detect and observe. Also this method has been used before to find hydrogen diffusion coefficients in different systems [1], [2]. The measurements were conducted at temperatures ranging from 2 K to 275 K at a pressure of 0.5 bars at 298 K, corresponding to a monolayer of H2 on our sample volume at 2 - 70K. The reason for measuring over such a large temperature range was to construct an Arrhenius plot which could be extrapolated up to realistic PEM fuel cell operating temperatures [3].

**Results from the experiment**
From the experiment we could indeed find diffusion coefficients on the surface of the carbon as well as other properties of the dynamics of the system. Fig. 1 shows how the experimental data fit the model of Chudley and Elliot, from 40, 50, 60 and 70 Kelvin for Q values up to 1.0 Å-1.

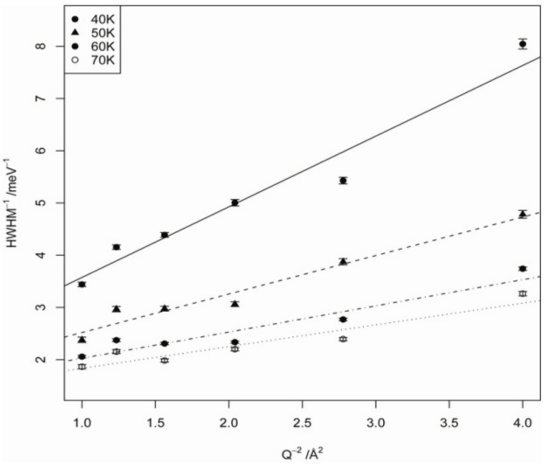

*Figure 1: Linearized data and fit.*

This figure shows the variation of the inverse of the measured HWHM as a function of Q-2. The values of the diffusion coefficients, D, the residence times, τ0, and jump lengths, l0, are presented in Table 1. The HWHM increases with increasing Q. The self diffusion coefficients found for 40, 50, 60 and 70 Kelvin are plotted in an

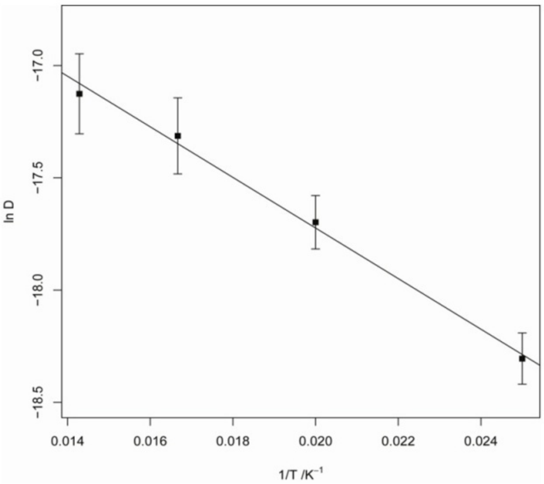

*Figure 2: Arrhenius plot of experimental diffusion coefficients.*

Arrhenius plot in Fig. 2. From the slope of the Arrhenius plot in Fig. 2 the D0 and E/kB coefficients was found to be, D0=1.9•10-7 ± 0.2•10-7 m2s-1and

E/k = 112 ± 5 K (1030 ± 50 Jmol-1). Comparing with liquid hydrogen which have the Arrhenius coefficients D0=8.58•10-8 ± 0.98•10-8 m2s-1and E/kB = 44.8 ± 1.6 K (372.5 ± 13.3 Jmol-1) [4]. Using these Arrhenius coefficients to estimate the change in the self diffusion coefficient at higher temperatures, we found a self diffusion coefficient of 1.4•10-7 m2s-1 at 398 Kelvin, a typical fuel cell temperature. In Fig. 4 the values of the natural logarithm of the surface diffusion coefficient, from this work together with the data from Bienfait et al. and Narehood et al. [5, 1], is plotted versus the inverse of the temperature are plotted.

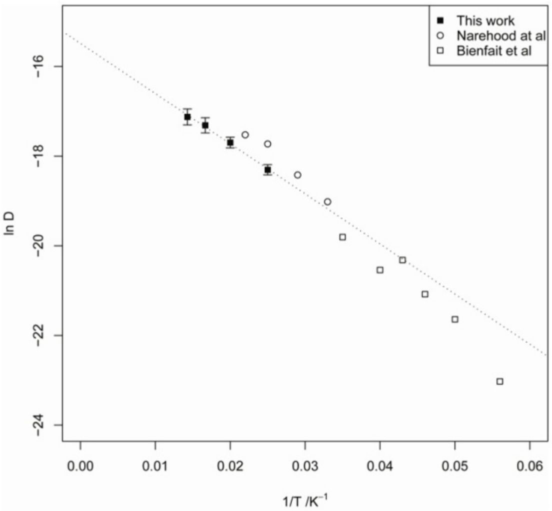

*Figure 3: Arrhenius plot of this work (full squares) together with that of Narehood et al. (open circles) and Bienfait et al. (open squares). They all show the same trend; the dotted line is the linear regression to our data.*

This work was done with collaboration with Peter Fouquet, Hannu Mutka and Stéphane Rols from the ILL, www.ill.fr.

Table 1: Parameters obtained from the fit of the Chudley and Elliot model to the experimental data at 40, 50, 60 and 70 Kelvin.

| T /K | $\tau_0$ /$10^{-12}$ s | Error /$10^{-12}$ s | D /$10^{-8}$ m2/s | Error /$10^{-8}$ m2/s | $l_0$ /$10^{-10}$ m | Error /$10^{-10}$ m |
|---|---|---|---|---|---|---|
| **40** | 1,5 | ±0,21 | 1,1 | ±0,13 | 1,3 | ±0,11 |
| **50** | 1,2 | ±0,13 | 2,1 | ±0,25 | 1,6 | ±0,10 |
| **60** | 1,0 | ±0,13 | 3,0 | ±0,51 | 1,7 | ±0,19 |
| **70** | 0,9 | ±0,11 | 3,7 | ±0,65 | 1,8 | ±0,21 |

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*Ole-Erich Haas, Signe Kjelstrup and Astrid Lund Ramstad, 2008.*

# Chemists are inspired by nature

Professor Signe Kjelstrup is on a quest to find inspiration for new, more energy-efficient chemical processes by studying nature. She need not look far, e.g. the human body is an impressive chemicals factory which engages in processes from which we can learn a great deal

Professor Signe Kjelstrup has studied energy conversion in natural and industrial systems for more than 20 years, and she has collected an imposing list of merits. She has, for example, headed the theoretical computation of a design for a distillation column that is 40 per cent more energy efficient than those currently used in the petroleum industry. The principle is shown in Fig.1. No less than 10 per cent of the USA's energy consumption goes to separating crude oil to produce fuel for cars in the US. Obviously, then, a more efficient distillation column could save huge amounts of energy and have an impact on the global climate.

For the moment, the new distillation column exists on paper only, but several foreign research groups have indicated their interest in the technology. The University of Delft in the Netherlands has appointed Kjelstrup to a professorship at the Centre for Sustainable Development. Moreover, the French industrial enterprise Air Liquide is interested in her technology and was recently granted funding through an EU project which aims to use the technology to develop a better process for air separation.

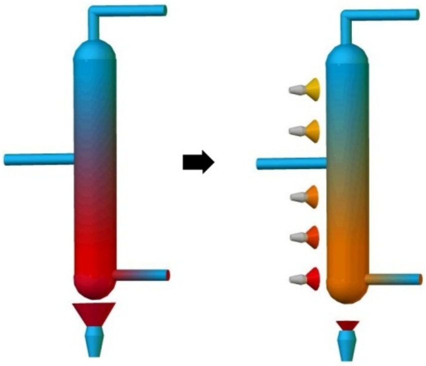


Fig.1. The conventional adiabatic distillation column (left) is much less energy efficient than the diabatic distillation column with distributed heating (right).

### Basic research and innovation

Kjelstrup's group will be working with innovation at the Centre for Advanced Study 2007-2008 from a platform based on the natural sciences. "We want to understand natural chemical processes better, and we believe that physics and mathematics will help us improve our descriptions of these processes. This may later lead to better models for energy optimal technical design. Otherwise, innovation is something that must take place in continuous interaction between scientists and users", points out Kjelstrup.

Professor Kjelstrup is especially interested in making theoretical descriptions of chemical processes, and the new distillation column is the result of a prolonged study of the processes at play when molecules in a liquid change and become a gas. The work was supported by the Research Council of Norway's Storforsk programme (Large-scale researcher-initiated projects), which was established to fund large-scale independent basic research projects entailing high risk and scientific boldness.

The development of the distillation columns has now progressed past the stage of basic research, and Kjelstrup is looking for new challenges. She has found one such challenge in the human body, which converts several kilos of chemical reagents to keep us going every single day.

### A molecular pump

"Cellular respiration in the human body and other organisms is a chemical reaction that takes place inside the cells. It involves converting glucose and oxygen to carbon dioxide, water and energy. The energy from this reaction is initially stored in a molecule called ATP (adenosine triphosphate). Synthesis takes place in the body's power plant, the mitochondria. The ATP molecule can, in fact, be part of a new chemical reaction that releases a high-energy phosphate ion, and this energy can then be used to run the different processes in the body's machinery. Just look, I'm lifting my arm, meaning I used a lot of ATP", continues Kjelstrup.

Kjelstrup and her colleagues have constructed a mathematical model of a large enzyme that uses the ATP molecule for an energy-intensive process. The enzyme is complex and weighs roughly the equivalent of 110 000 hydrogen atoms. "Ca-ATPase, as the enzyme is called, is quite simply a sort of molecular pump, in the sense that it pumps calcium ions up to higher energy levels. We are trying to understand this pump, which consists of a single molecule and is capable of transforming chemical energy for the transportation of ions. This is a highly efficient chemical process. If we can understand it better, we may possibly be able to use the knowledge to develop other effective chemical processes at the nano level", postulates Kjelstrup.

A better understanding of the Ca-ATPase molecule could give us new insight into obesity, a growing problem in many affluent countries. "Obesity and overweight are associated with the body's ability to regulate heat and work, and there is a good chance that it is calcium pumps that regulate those functions. We believe that Ca-ATPase is a heat pump in addition to being an ion pump", suggests Kjelstrup.

### A brain heater

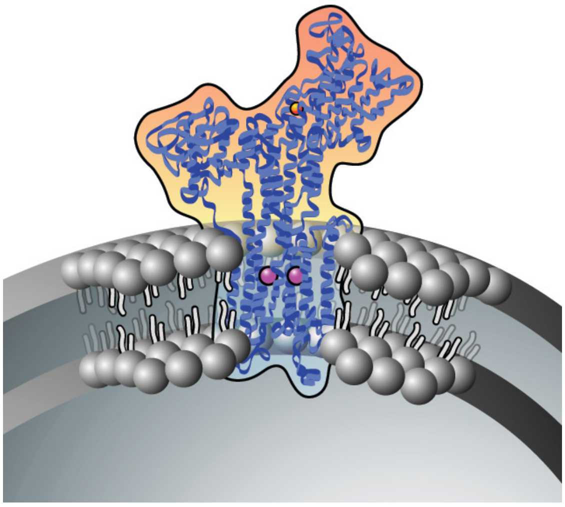
Ca-ATPase is found not only in the human body, but also in the vast majority of living organisms, including animals and bacteria. Professor Kjelstrup's co-workers have found an especially interesting application of Ca-ATPase in the brain of swordfish, which often dive down to great depths in waters down to temperatures of 4 °C to hunt for prey. The swordfish brain would have functioned poorly at such low temperatures, had it not contained a sort of electrical heater that turns on automatically when the fish dives down into the briny deep. Humans and many other animals can stay warm by increasing muscular activity, for example, by flailing their arms or shivering. Swordfish, on the other hand, gear up their brain metabolism.

Professor Kjelstrup is heading the research group Chemical process design inspired by nature at the Centre for Advanced Study in 2007-2008. The group will spend the autumn semester concentrating on gaining a better understanding of ion pumps, especially Ca-ATPase. "We believe we can use that knowledge to design better chemical processes in general. During the spring semester, we'll take a closer look at the reaction between hydrogen and oxygen in fuel cells. The common denominator between the ATP project and the fuel cell project is that we need to develop a better understanding of the processes and a thermodynamic description at the nano level", adds Kjelstrup.

Mathematics is the language of nature, and Professor Kjelstrup uses mathematical modelling as an important tool. The mathematical computations for modelling are sometimes heavy-going. It helps that the CAS group has access to computing resources at Riken research institute in Japan, Imperial College in England and the Spanish supercomputer system Mare Nostrum in Barcelona.

Kjelstrup's computer contains a model of Ca-ATPase that shows how the 'pump' vibrates before abruptly spitting out a high-energy calcium ion from the one end. Vibrations occur at the pico-second level, i.e. vibrations take about 0.000000000001 second. But the calcium transport takes milliseconds. It is a great problem to link these scales.

"It is fantastic to get be at CAS for a whole year. We will have a unique opportunity to delve deeply into details. During the course of this year, I hope that we will manage to develop some methods that we can use for research in the decades ahead", reports Kjelstrup.



*Ca-ATPase is a molecular pump that pushes calcium ions up to higher energy levels. The pump vibrates at a rate of about 0.000000000001 second (1THz), but it transports ions on a millisecond scale.*

*Professor Signe Kjelstrup is Head of the Research Group "Chemical process design inspired by nature", at the Centre for Advanced Studies. Signe is on leave from the Department of Chemistry.*

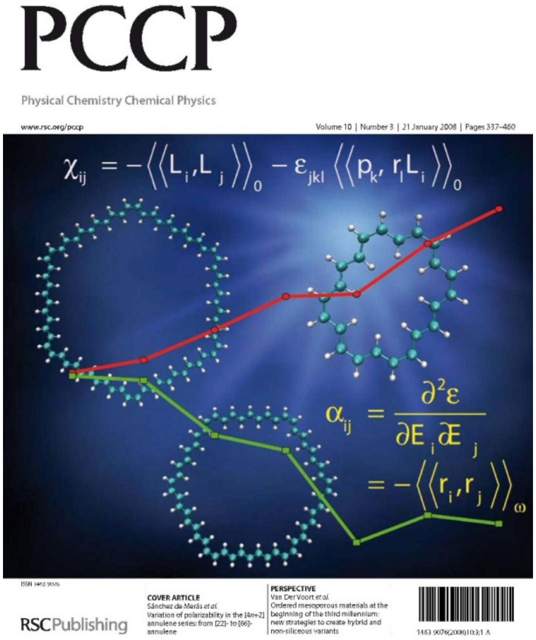
*Signe Kjelstrup*

# Variation of polarizability in the [4n + 2] annulene series: from [22]- to [66]-annulene

Using correlated ab initio methods, the polarizability of large [4n þ 2]-annulenes is determined, showing that there exists an almost linear relation between the exaltation of magnetic susceptibility (a measure of aromaticity) and an equivalent enlargement of polarizability.

## Introduction

According to the pioneering definition by Sondheimer,[1] annulenes are fully conjugated hydrocarbon monocycles. Benzene, [6]-annulene, in addition to being the most prominent aromatic molecule, is the smallest representative of the neutral [4n + 2] series, while cyclobutadiene represents the absolute smallest annulene. Like benzene, annulenes have been extensivelyused as model systems to study aromaticity. In fact, the last decades have seen a renewed interest in this kind of compounds, partly motivated by a number of synthetic findings. Moreover, [4n + 2]-annulenes may serve as prototypes of one-dimensional metals[2] and some annulenes show very interesting properties from a nanotechnological perspective.[3] Forinstance, Pak et al. have reported a series of site-specific electron-donor and/or acceptor-functionalized [18]-annulenes,[4] some of them presenting nonlinear optical properties.[5] In addition, dehydrobenzo[20]annulenes can form ordered onion- and tube-type nanostructures.[6] For some recent review on the chemistry of annulenes, see the paper by Haley and coworkers.[7] All these findings make research in this kind of systems very interesting. In this context, theoretical methods provide a cheap way of predicting such properties, including molecules of higher molecular weight. Among these properties, polarizability has an essential function in a variety of physical and chemical processes. In this work, we report an ab initio study of static and dynamic polarizabilities of [4n + 2]-annulenes for n = 5, 6, 7, 10, 13, and 16 computed using a CC2 linear response approach.[8]



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**COVER ARTICLE**
Sánchez de Merás *et al.*
Variation of polarizability in the [4*n*+2] annulene series: from [22]- to [66]-annulene

**PERSPECTIVE**
Van Der Voort *et al.*
Ordered mesoporous materials at the beginning of the third millennium: new strategies to create hybrid and non-siliceous variants

1463-9076(2008)10:3;1-A

*Cover page of Physical Chemistry Chemical Physics, vol.10, no.3, Jan.2008.*

## Conclusions

We have reported the polarizabilities of large [4n þ 2]-annulenes in both localized and delocalized structures computed at the CC2/aug-cc-pVDZ level of theory. As in the case of small annulenes, we have found a linear behavior of the perpendicular component of the polarizability with respect to the number of double bonds. Moreover, an almost linear relationship between the exaltations of magnetic susceptibility and electric polarizability has been determined.

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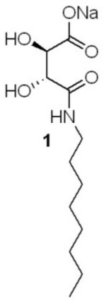
*Henrik Koch*

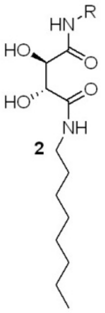
# Optically Active Amphiphiles

Cell membranes, nucleic acid multiplexes, proteins and protein complexes with nucleic acids or membranes and the function of enzymes are due to supramolecular assemb-lies that consist of mesoscopic superstructures in the 10-1000 nm size range. They are spon-taneously self-assembled into these structures due to non-covalent interactions such as elec-trostatic-, dipole-dipole interaction, hydrogen bonding, dispersion-, and hydrophobic forces. Controlled and directed self-organization through mastering the non-covalent interact-tions is an important instrument for the control at the molecular level.

We synthesize and study the behavior of amphiphilic compounds, which are struc-tures containing both a hydrophilic and a hydrophobic part. Typical examples of amphi-philes are the lipids found in biologic mem-branes. In biologic systems most molecules are chiral. Chirality is therefore an important factor for the understanding of how such systems self-assemble into superstructures. Optically active amphiphiles are therefore components of interest for the use in supra-molecular chemistry and for the fabrication of micelles, liposomes, vesicles and membranes. Many of these find practical applications in for instance time controlled delivery systems of therapeutic agents, for transport of genetic material, ultrasound diagnostic, production of nano-sized particles, semiconductors, electro-optical devices, metallic and magnetic nano-materials and for separation methods.



1



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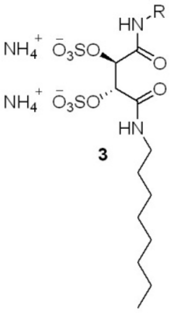


3

Our work was focused on the supramolecular chemistry of optically active amphiphiles. Tartaric acid was selected as the general source of chirality. All of the tartaric acid stereoisomers are inexpensive and readily available. The studies concentrated on the hydrolytically robust amide derivatives, such as analogs of N-mono-alkyltartramides, N,N-di-alkyltartramides, and the more soluble disul-fates. Representative constructions are struc-tures 1-3. These compounds were all predicted to be readily biodegradable.

Syntheses were developed for the construction of a number of such systems, in which the alkyl substituents were varied together with the chirality of the tartaric acid portion of the molecules. The surface active properties of these products have been studied together with how they assembled into micelles and vesicles.

Light microscopy showed that they may formed vesicles, for example cell-like structures or liposomes, as shown in Figure 1.

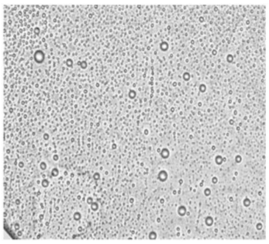


Figure 1

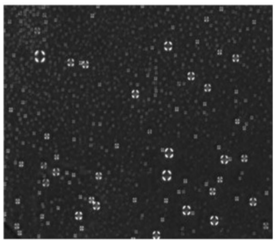


Figure 2

Using polarized light microscopy, Figure 2, the characteristic “Maltese cross" was observed, indicating an anisotropic nature of the vesicles.

For some of the monoamides of type 1, interesting dynamic vesicle behaviour was observed. Thus, one product initially formed spherical vesicles which, however, upon standing “buds”, which grew into spiral formed vesicles, Figure 3.

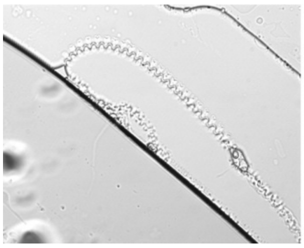


Figure 3


Figure 4

The structures of the vesicles have also been studied by Transmission Electron Micro-scopy, SEM. In Figure 4 is shown a SEM picture of an aggregate formed from an amide of type 1. The vesicle was grown in a neutral buffer solution, and clearly shows formation of a laminar structure.

Studies of amphiphiles of type 2 and 3 are currently in progress. They exhibit promising properties which are investigated in collabora-tion with a group at University of Perugia, Italy.

*Susanna Villa Gonzalez, Qiang Yu and Per Carlsen*

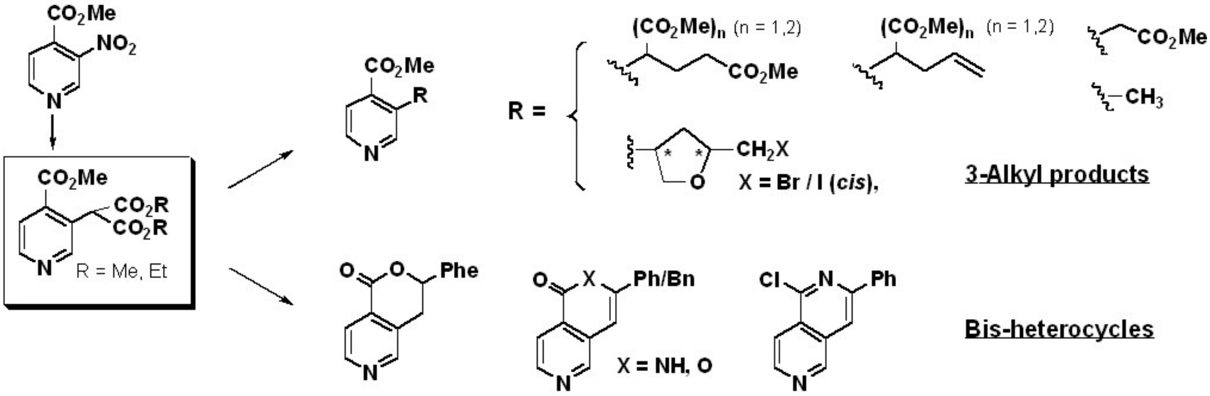
## The Nitropyridine group

**Background:**
In heterocyclic chemistry pyridines are essential, being one of the most abundant and best known groups of aromatic heterocycles. The pyridine ring system is incorporated into the structure of pharmaceuticals, natural products, agrochemicals, ligands in transition metal catalyst complexes and commercial products. Nitro-pyridine derivatives are suitable substrates for the preparation of novel heterocyclic products; many of these heterocyclic systems may have biological activity.

- We are investigating the chemistry of nitropyridine derivatives.
- We utilize nitropyridines derivatives as substrates for the formation of new products with potential biological activity, including bis-heterocycles.
- We are developing new synthetic routes to fused heterocycles.

**1. Pyridyl malonate chemistry**
*Tjosås, F.; Pettersen, N. M.; Fiksdahl, A. "α-(3-Pyridyl)malonates; Preparation and Synthetic Applications",*
*Tetrahedron 63(48) (2007) 11893*

Alkylation of aromatic rings is a major challenge in organic syntheses since more complex carbon skeletons can be constructed. The alkylation of pyridine by nucleophilic aromatic subst. of the nitro group in methyl 3-nitro-4-pyridylcarboxylate by malonic ester was successful. The versatility of the α-(3-pyridyl)malonate product was demonstrated by the formation of a number of novel compounds:



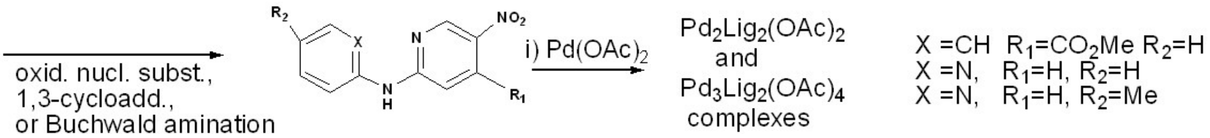
The results demonstrate that the nitropyridine- α-pyridylmalonate pathway may represent a convenient strategy both for the preparation of 3-alkylpyridines and more complex carbon skeletons, such as fused bis-heterocycles.

- *The synthetic potential of the nitropyridyl substrate is thus demonstrated.*

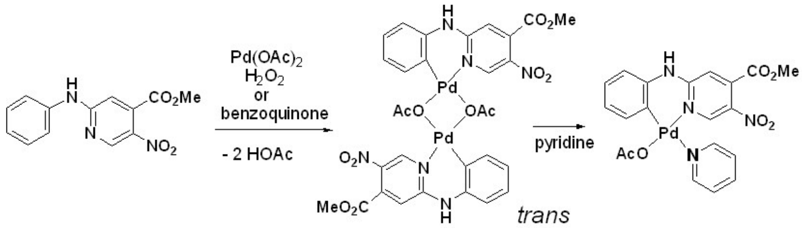
## 2. Palladium complexes

*Tjosås, F.; Fiksdahl, A.; "Palladium complexes of N-aryl-2-pyridylamines" J. Organomet Chem. 692 (2007) 5429.*
*http://dx.doi.org/10.1016/j.jorganchem.2007.09.002*
*Hansen, L. K.; Tjosås, F.; Fiksdahl, A. Acta Cryst. E62 (2006) o3728-o3729.*

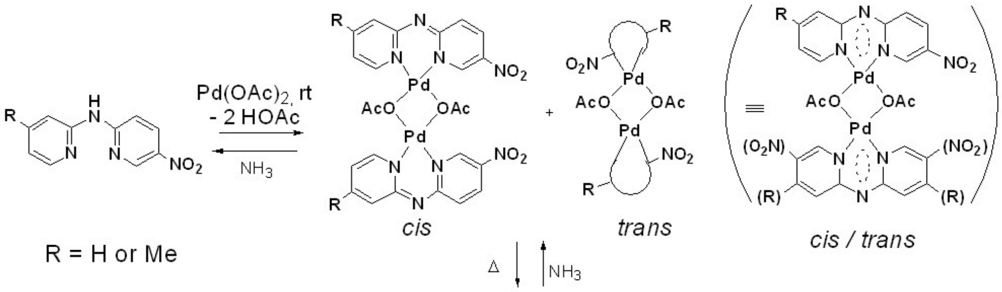
*N*-Aryl-2-pyridylamines were prepared. Due to the coordination ability of the pyridine-nitrogen atoms, a number of PdII complexes (i), ii) below) were isolated when the pyridyl substrates were subjected to $Pd(OAc)_2$ complexations.



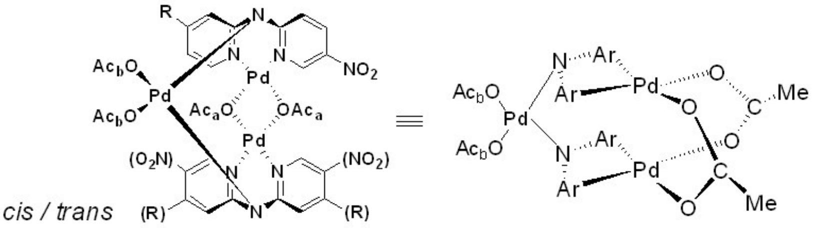
**i) *N*-phenylpyridylamine:**
A new method for the preparation of the *acetato-bridged 6-membered ring palladacycle complex* was developed:



**ii) Dipyridylamines:**
formed
*cis/trans bis-dentate acetato-bridged dimeric $Pd_2Lig_2(OAc)_2$*
at room temperature:



and subsequently
*cis/trans $Pd_3Lig_2(OAc)_4$ complexes*
by heating:



NMR and ESI-MS was used for determination of complex compositions. $^1H$ and $^{13}C$ NMR characterisation of all the individual *cis* and *trans* isomers of bis-dentate acetato-bridged dimeric $Pd_2Lig_2(OAc)_2$ and $Pd_3Lig_2(OAc)_4$ complexes are reported.

*Anne Fiksdahl*

# The Fluoro-organic group: Synthesis and utilization of α-fluoroacetophenones

**Background:**
The importance of fluorinated compounds in relation to pharmaceuticals, agrochemicals and material sciences has been thoroughly recognised. As a consequence fluorinated building blocks are required. The current work is the starting point of a technology platform for synthesis of new biological active compounds based on already existing hydrogen analogues.

## 1. Synthesis of α-fluoroacetophenones

*Erik Fuglseth, Thor Håkon Krane Thvedt, Bård Helge Hoff; submitted.*

Being in need of a series of α-fluoroacetophenones, it was recognised that literature mainly covers reactions toward the parent compound 2-fluoro-1-phenylethanone (**1c**), and few systematic studies on effect of substrate structure on yield had been performed. The aim of this work was to compare electrophilic and nucleophilic fluorination using Selectfluor (F-TEDA-BF4, 1-chloromethyl-4-fluoro-1,4-diazoniabicyclo[2.2.2]octane bis-(tetrafluoroborate)) and tetrabutylammonium hydrogen difluoride (TBAHF2) for the synthesis of α-fluoroacetophenones.

The yields of all routes were affected by substrate structure. In general, electrophilic fluorination of trimethylsilyl enol ethers (Route A), gave higher yield than for the other methods tested. Route B was advantageous in terms of simplicity, however prolonged reaction times limits its usefulness. Nucleophilic fluorination (Route C) is not competitive with electrophilic strategies due to low yield especially when electron withdrawing R-groups are introduced. The loss in yield is mainly due to condensation reaction of the Aldol and Darzen type.

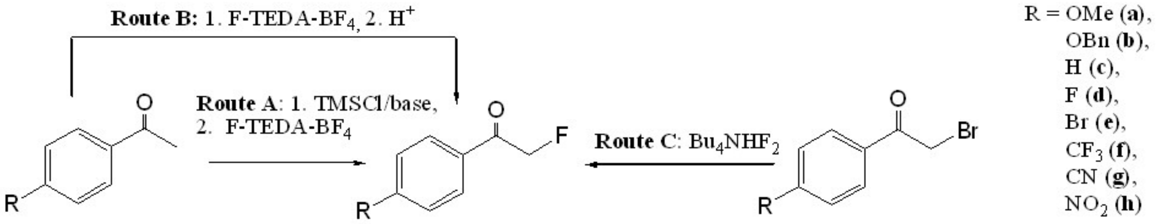


*Figure 1. Routes tested for synthesis of α-fluoroacetophenones.*

## 2. Asymmetric reduction of α-fluoroacetophenones

*Erik Fuglseth, Eirik Sundby[a], Bård Helge Hoff; manuscript in preparation*
*[a] Sør-Trøndelag University College, Faculty of Technology, N-7004 Trondheim, Norway*

Enantiopure compounds are of uttermost importance when dealing with biological active molecules. Asymmetric reduction of the prochiral fluoroketones leads to enantioenriched 1,2-fluorohydrins. Reduction using the proline base catalyst (*R*)-MeCBS, has been optimised with respect to reaction solvent, addition rate and reaction temperature. The optimised conditions were then compared with the performances of Bakers yeast (*Saccharomyces cerevisiae*) and *Geothricum candidum*.

All the 1,2-fluoroalcohols were synthesised in decent yields and with good to excellent enantiomeric excess. Six of these compounds have not been described in prior literature. The three reaction systems tested all gave a preference for the *R*-enantiomer, and is complementary if a high ee-value is the main target. The biocatalysts are easier to prepare than (*R*)-MeCBS. However, conversion rates and dilution factors favours the use the (*R*)-MeCBS system.

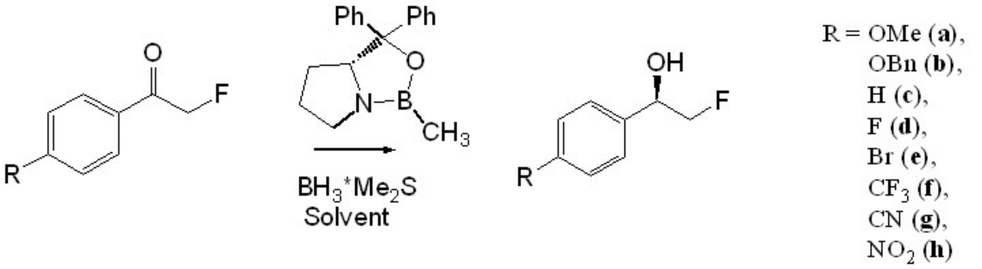


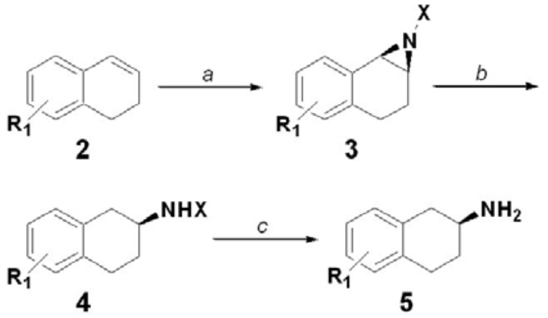
*Figure 2. Asymmetric reduction using (R)MeCBS catalyst.*

*Bård Hoff*

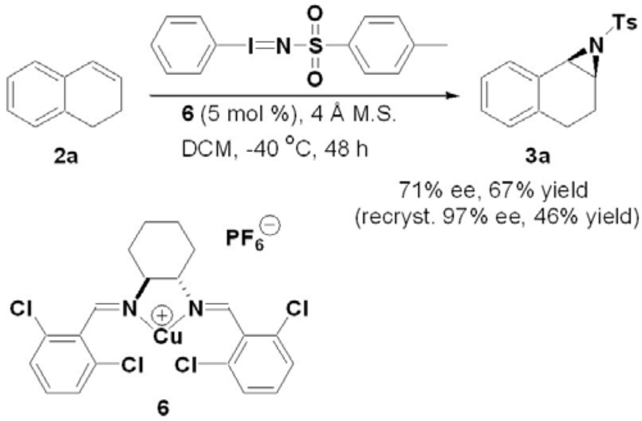
## Asymmetric catalytic aziridination of 1,2-dihydronaphthalenes

(Melnes, S.; Aaseng, J. E.; Reian, G.; Gautun, O. R. to be published)

Numerous articles have been published during the past years concerning 2-aminotetralins **5** and their use as physiologically active reagents.[1] However; no cost-efficient routes to optically pure **5** exist today. We are currently working with a general three steps method for preparation of different substituted and optically active **5** as shown below. The challenging step in this protocol is step a involving asymmetric aziridination of 1,2-dihydronaphthalenes **2**.



Several known catalytic systems for asymmetric aziridination have been tested using PhI=NTs and PhI=NNs as nitrene donors. The best results were obtained using Jackobsen's catalyst **6**.[2]

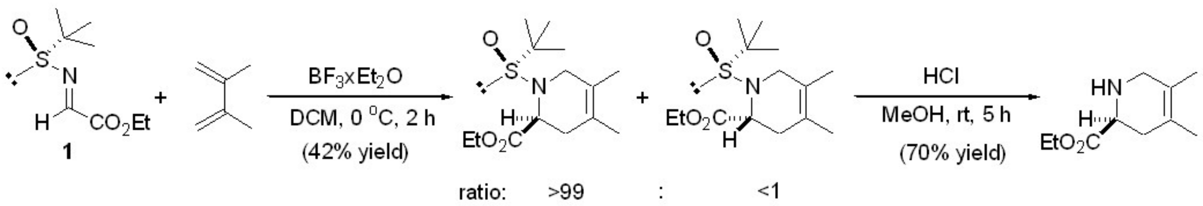


1) A SciFinder search of "2-aminotetraline" and "2-aminotetralin" gave more than 1800 hits, of which most concerns physiological properties of the compounds.
2) Li, Z.; Quan, R. W.; Jacobsen, E. N. *J. Am. Chem. Soc.* **1993**, 115, 5326.

## Asymmetric aza-Diels-Alder reactions

(Andreassen, T.; Håland, T.; Hansen, L. K.; Gautun, O. R. "*Asymmetric aza-Diels-Alder reactions of an N-tert-butanesulfinyl α-imino ester", Tetrahedron Letters* **2007**, *48*, 8413)

The aza-Diels-Alder (aza-DA) reaction of imino dienophiles is a powerful tool for the rapid construction of highly functionalised six-membered nitrogen heterocycles such as piperidines and tetrahydroquinolines. We have demonstrated that optically active *N-tert*-butanesulfinyl α-imino ester **1** reacts with both activated and non-activated dienes in presence of $BF_3 \cdot OEt_2$. The aza-DA adducts were obtained in modest yields and in diastereoselectivities ranging from poor for the activated Danishefsky type dienes to excellent for the unactivated acyclic dienes (up to 99% de).



The configurations of the aza-DA adducts were established either by X-ray analysis or by chemical correlation to known compounds.

*Odd Reidar Gautun*

# Carotenoids and genes in the Middle East

**The group of Professor Vassilia Partali has been working on hydrophilic carotenoid derivatives for more than a decade and much progress have been made since the first experiments. The objective was originally to increase bioavailability and areas of application of the carotenoid derivatives. After being contacted by assistant Professor Michael D. Pungente at *Weill Cornell Medical College in Qatar* (WCMC-Q), attention was shifted towards synthesising cationic carotenoid derivatives for gene therapy experiments.**

**What is gene therapy?**

Gene therapy is basically described as the intracellular delivery of genetic material to generate a therapeutic effect by correcting an existing abnormality or providing cells with a new function. Chemically based delivery systems (hereunder cationic derivatives) are found to be the safest method for this treatment, and much effort is put into making the cationic derivatives more efficient.[1]

Being a master-student and now a PhD-student and get to work on this project has been both challenging and rewarding. When I was invited to go to WCMC-Q in June 2007 to supervise the first preliminary gene-therapy experiments and also present the development of these compounds this co-operation was finally concretised.

WCMC-Q is a joint initiative between the Qatar government and WCMC which has an objective to increase international influence. This is a result of Qatar's aggressive work to improve the academic quality, and it is also obvious in the fact that more than 4.5% of the GDP is used for research and academic purposes every year.[2]

*Working in the lab. From right: Dr. M.D. Pungente, D. Vijayakumar, S. Joseph*

During my stay in Qatar I was given the privilege to supervise two students in the pre-medical program in the preliminary experiments with the compounds I had synthesised at NTNU. We were testing out methods to analyse the compounds' affinity to DNA, and their abilities to protect the DNA from harmful effects that can be present in an organism. The results from these experiments were very promising, and they are at present being reproduced for validation.

Dr. Ronald Crystal, who is acknowledged as one of the leading authorities in the field of *in vivo* gene therapy, was visiting the university while I was there. Dr. Pungente was kind enough to arrange a meeting with Dr. Crystal, and we discussed the future potential of the project and also the possibility of extending the project further. Dr. Crystal was positive to the thought of conducting *in vivo* experiments with the cationic carotenoid derivatives if the preliminary results from WCMC-Q were promising.

*From right: Dr. M.D. Pungente, Dr. R. Crystal, S. Joseph, D. Vijayakumar, C.L. Øpstad*

Being a country in the Middle East, Qatar still suffer from many limitations when it comes to rapid delivery of necessary chemicals or easy access to spectroscopic equipment. In many cases the universities and research institutions have to turn to one another in order to get their results, as I also experienced on several occasions.

*The campus of WCMC-Q in Education City, Doha*

A research seminar was held in conjunction with my visit at the university. Scientific staff and students from WCMC-Q and other universities were invited to attend, and I held a lecture entitled; "*Carotenoids, Antioxidants and Novel Gene-Transport Vectors*". Light lunch was served at the seminar, and after the lecture we discussed details of the research as well as the potential of these compounds as therapeutic agents.

In addition to working at the university I also spent some time exploring Qatar and the capital, Doha. The country is a melting pot of different cultures, and the strictly Muslim way of living is neatly combined with the more western lifestyle of many people. In Doha there are malls beyond imagination and breathtaking buildings are being built all over the city. Just a short drive from the busy capital is the desert which dominates the Arabian Peninsula. A desert safari with dune-surfing and dinner in nomad-tents at the beach was absolutely worth experiencing.

*Downtown Doha, Sheraton Hotel in front.*

The benefit of this trip was both the scientific results we obtained in the preliminary experiments, as well as establishing a more formal co-operation between the group the researchers at NTNU and at WCMC-Q.

**The cationic carotenoid project**

This project is highly interdisciplinary, and combines elements from organic chemistry, physical chemistry, physics, biology, biotechnology and medicine. In addition to giving the opportunity to get a broader platform of expertise it also gives a common basis for colleagues from different backgrounds to cooperate.

The involvement of several departments at NTNU in addition to international collaborators makes this project significant, especially with regard to future development.

The use of these compounds is not restricted to gene therapy purposes, and may also prove important in other areas of use, i.e. drug carriers or food colorants.

*Al-Wakhra, The inland sea*

*Christer L. Øpstad, PhD-student*

References:
[1]Lemoine N.R. (Ed.), *Understanding Gene Therapy*, Springer, New York, 1999.
[2] The WCMC website:
http://www.cornell.edu

*Going to Qatar was a great experience!*

# BLUE / GREEN MACROCYCLES Studies of azaphthalocyanine derivatives

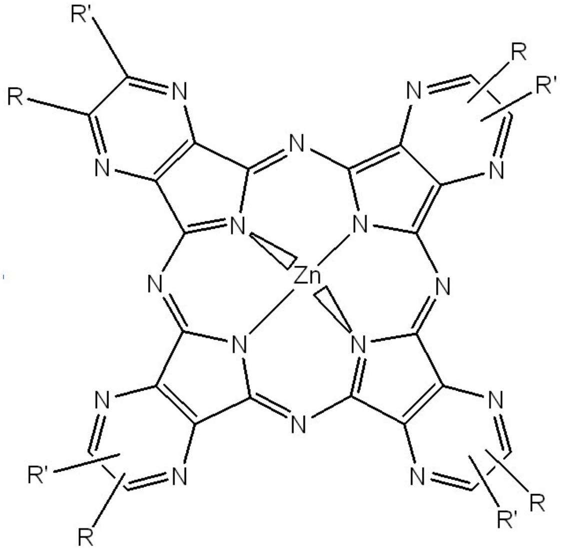
Phthalocyanines (Pcs) are some of the best known industrial pigments, and are produced in thousands of tons every year to meet the demand for blue and green colorants. The phthalocyanine structure consists of an aromatic 18 B-electron system. Metal complexes of Pcs can be formed with various metal ions, and substituents may be introduced to the periphery of these macrocycles in order to alter characteristics such as solubility, colour and aggregation.

Whereas Pcs have been subject to extensive studies for almost a century, the analogous azaphthalocyanines (AzaPcs) are less known, but may be of even more interest for various applications.

Several years ago, when AzaPcs caught our interest, we found that synthesis of heteroatom (O, N, S) substituted AzaPcs was not straight forward. The synthetic scheme involves cyclotetramerisation of substituted pyrazine-2,3-dicarbonitriles as monomers. Some substituents were labile, i.e. were exchanged with the strong nucleophiles used during the cyclotetramerisations, whereas other types of substitutents hindered formation of AzaPcs due to strong electron donation. Carbon- bound substituents eliminated some of the synthetic problems, but targeted characteristics of the AzaPcs were not obtained in some instances. When unsymmetrically substituted pyrazine-2,3-dicarbonitriles are used, four constitutional isomers of AzaPcs can be obtained, and such isomer mixtures may be of special interest.

Presently we are studying AzaPcs of potential use in photdynamic therapy (PDT), or as diagnostic markers for medical purposes. Important characteristics of such compounds are: good solubility in organic solvents, low tendency to aggregation, major UV-vis absorption at approximately 700 nm. In addition the compounds should preferably be efficient sensitizers for singlet oxygen formation – or show strong red fluorescence in the near-IR region.

Our recent efforts towards these goals are shown in the enclosed list of publications. Both symmetrically and unsymmetrically substituted AzaPcs have been prepared, and some substitution patterns show good promise for further studies.



*Unsymetrically substituted zinc-azaptalocyanine*

*Eva H. Mørkved*

## Mercury speciation in the Norwegian arctic seasonal trends and (bio-) availability of deposited mercury

During spring 2007, Torunn Berg (professor) and Anne Orderdalen Steen (Ph.D student) started continuous mercury speciation measurements at Ny-Ålesund, Svalbard. The project is funded by the the Norwegian Research Council (NFR) (MILJØ2015) and is an important contribution to the International Polar Year (IPY).

The aim of the project was to study so-called "Atmospheric Mercury Depletion Events" (AMDE.). About 95% of the total atmospheric mercury is normally gaseous elemental mercury GEM). During polar spring, however, a drop in the level of GEM is seen. This is due to oxidation of GEM to more reactive mercury species, which are absorbed on particles. AMDE was first observed in the Canadian Arctic in 1995 (Schroeder *et* al. 1998), at Ny-Ålesund in 2000 (Berg et al. 2003). Simultaneously with the drop in GEM elevated levels of the reactive mercury forms are observed. The oxidation take place only during a few month period after polar sunrise and the reactive mercury forms are deposited to the snow covered surfaces. This may explain elevated mercury concentrations in Arctic marine food webs.

NTNU's speciation data for 2007 is the longest time series which ever have been measured at Ny-Ålesund as well as for other measurement sites in the European Arctic. This work have resulted in knew insight into this spectacular phenomenon. The overall budget for mercury at Ny-Ålesund was studied: Snow as well as fluxes of mercury between snow/soil and the atmosphere were analysed. Increased mercury concentrations in surface snow were observed during and after AMDE events, a result of deposition of reactive species of mercury from the atmosphere. Parts of the mercury in the snow were reemitted back to the atmosphere.
Further research is necessary to improve the knowledge on AMDE and the Arctic mercury budget, and a new campaign will be carried out at Ny-Ålesund in March-August 2008.

*Photos: Torunn Berg, Ida Beathe Øverjordet and Anne Orderdalen Steen*

*Anne Orderdalen Steen and Torunn Berg*

# Trace elements in cerebrospinal fluid and blood from patients with Skogholt's disease, a rare neurodegenerative disease in Norway

A family with a rare neurological disease has recently been discovered in Hedmark county in Norway. The disease shows some similarity to multiple sclerosis, but also affects the peripheral nervous system, and is different from other similar disorders described in the literature (1,2). Thus, it seems that this is a distinct disease entity, and it has been named Skogholt's disease, after the local physician who first discovered the disease among members of this family. The disease has so far been diagnosed in 3 generations (Figure 1). The symptom onset varies from before 30 to after 50 years of age, and the disease is gradually progressive. Causes and mechanisms of this disease are unknown. Therefore, in collaboration with Dr. Skogholt and Sykehuset Innlandet (the hospitals in Kongsvinger and Elverum), we decided to investigate the possible role of trace elements in this disease.

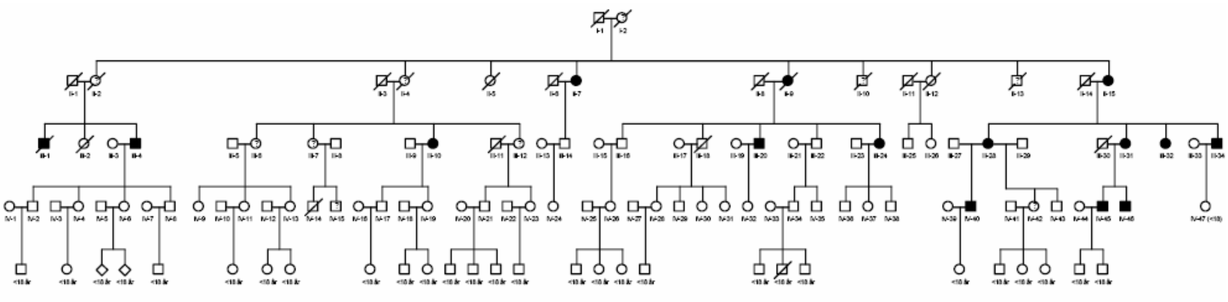


*Figure 1. Pedigree (family tree) for the family with Skogholt's disease, showing the last 5 generations. Our study includes patients from generations II, III and IV. Squares indicate women, circles indicate men, dark fields indicate disease (certain) and angular lines indicate that the person is dead. The figure is from Annette Skogholt's M.Sc. thesis (2).*

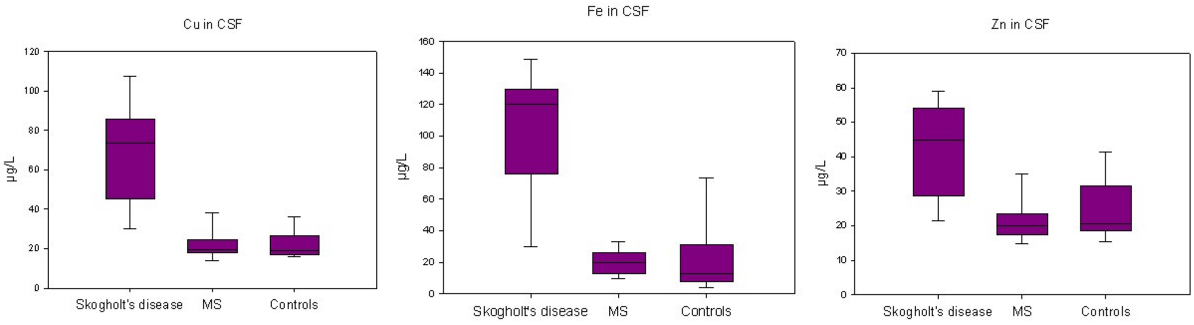


*Figure 2. Concentrations of copper, iron and zinc in cerebrospinal fluid (CSF) from 10 Skogholt patients, 9 multiple sclerosis (MS) patients and 13 controls.*

Trace elements influence human health by a host of different mechanisms. Trace elements, and especially some transition metals, have been implicated in the development of several neurodegenerative diseases. All 10 Skogholt patients who were physically capable of travel to the hospital volunteered for sampling of cerebrospinal fluid (CSF) and blood. We also included 9 subjects diagnosed with multiple sclerosis and 13 individuals with no known neurological disease (the control group) in the study. The concentrations of 31 elements were determined by HR-ICP-MS in CSF, blood plasma and whole blood from all participants (3).

The main finding in our study was extremely high levels of Cu, Fe and Zn in CSF from patients with Skogholt's disease (Figure 2). All these three metals are known to bind to proteins in biological fluids. One of the distinct characteristics of Skogholt's disease is a highly increased protein level in the CSF, which was confirmed in this study. The increased protein level is probably due to a leakage defect in the blood-brain barrier (1). Thus, based on our results we hypothesize that a blood-brain barrier dysfunction is an early and presumably primary inherited defect, which causes the observed increases in metal concentrations (3). The resulting long-term exposure to increased metal levels may then contribute to brain tissue damage in Skogholt's disease.

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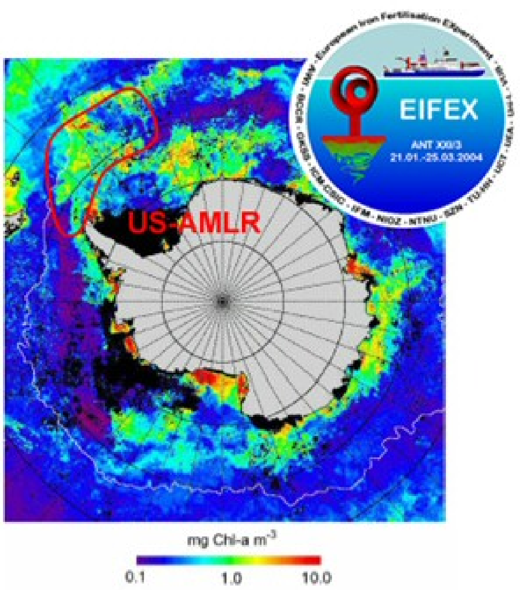
3. Gellein K, Skogholt JK, Aaseth J, Thoresen GB, Lierhagen S, Steinnes E, Syversen T, Flaten TP. Trace elements in cerebrospinal fluid and blood from patients with a rare progressive central and peripheral demyelinating disease. *J Neurol Sci* 2008; **266**: 70-78.

*Kristin Gellein and Trond Peder Flaten*

# The role of Iron in Biological Production and the Carbon Cycle in the Southern Oceans (NPI/ NFR project)



In the beginning of 1990s the ‘Iron Hypothesis’ lead to a radical paradigm shift in marine science. Prior to the iron hypothesis, many oceanographers were quite skeptical about large scale *in situ* enrichment of a patch of open ocean water with an element. Now, marine scientist are not just collecting samples and observing the oceans, but they have jointly started to perform mesoscale *in situ* experiments in various oceans in order to understand the effects of iron on biological processes and C cycles.

From 1993 to 2004 there have been 12 large scale iron enrichment experiments in different Oceans. These experiments and previous iron measurements have unequivocally shown that iron is the limiting element for biological production in almost one-third of the world ocean. Besides, iron supply controls also the biological pump, with the effect of drawing down the atmospheric $CO_2$ level both in glacial periods and in modern days.

Due to the recent revelation of Iron´s crucial role in the biogeochemical cycles of carbon, nitrogen and sulfur and ultimately the Earth climate, Iron studies became hot topics in the climate and biogeochemical studies in marine science

In close cooperation with IBI/TBS we started iron research in coastal waters in 1995 (1; 2) and in the Southern Ocean, Antarctica, in 1997 (3 ;4). We participa-ted in the largest and longest iron enrichment experiment (EiFEX) in the Southern Ocean in 2004 (5; 6). In 2006, 2007 and 2008 we have actively been involved in US-NOAA AMLR program that focuses on the coastal waters of Antarctica, Weddell Sea and Antarctic Circumpolar Current systems, aiming to understand the role of natural enrichment of iron on the biological productivity in these regions. In Norway, NTNU is the only institute performing research in this newly emerging area, in corporation with prominent international research groups.

We have recently started a collaboration with Chilean scientists aiming at the investigation of the interaction between macro nutrient rich and iron poor southern Humboldt current and the Chilean fjord system. Related to this, we have performed a short cruise and incubation experiment in December 2007 in Chile.

Additionally a mesocosm experiment has been performed (in autumn 2007) at the TBS research pool to test the effects of the organic matter on the iron bioavailabilty for phytoplankton, with collaboration with Turkish and Germen marine scientists.

References:

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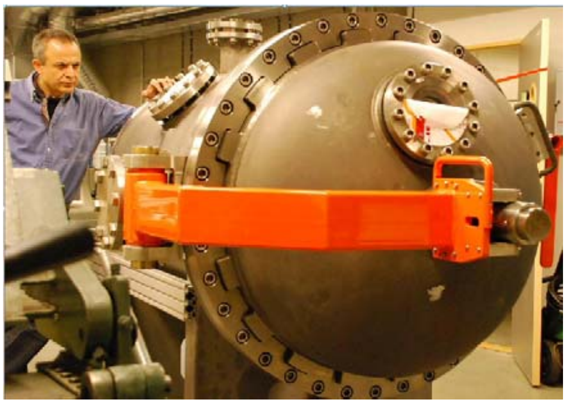
*Murat V. Ardelan (previously M. Öztürk)*

# Changes in trace metal biogeochemistry in the sediment and sediment-water interface following $CO_2$ seepage from saline aquifers (VISTA project).



The $CO_2$-affected global warming and the means for environmentally acceptable disposal of $CO_2$ has been a hot topic in recent years. One of the mitigation measures that has eagerly been suggested is the injection of large amounts of $CO_2$ into deep saline aquifers.

In the North Sea a pioneering injection program has been carried out by the STATOIL company since 1996 at Sleipner Vest. The success of this disposal strategy is dependent on the permanent retention of $CO_2$ in the aquifer. Therefore, the likelihood of the leakage of some fraction of the stored $CO_2$ into the overlaying sediment and the seawater as well as the possible effects associated with such a leakage need to be studied.

The leaking or seeping of $CO_2$ into the sediment-water interface and further into the deep seawater may lead to a cascade of biogeochemical alterations with detrimental effects in the marine systems. A possible $CO_2$ leakage from geological storage sites into the surface sediment and to the deep sea may cause a metal release to the pore water of the sediment and the sediment-water interface, followed by an enhanced metal flux to the water column. The acidic conditions due to CO2 seepage may effect dissolution and/or desorption of potentially hazardous trace metals harming marine organisms.

In 2006-2007 we developed a lab-scale non-pressurized reactor/chambers. We performed a number of small-scale tests involving a direct release of $CO_2$ in a non-pressurized reactor in order to obtain data related to the possible effects of $CO_2$ leakage on trace metal geochemistry in the sediment-water interface. Preliminary experimental results have been submitted for publication (1;2).

As a main part of this project, a high pressure tank has been built exclusively in titanium, financed by STATOIL. For testing the biogeochemical effects of $CO_2$ seepage under high pressure, we will perform our experiments also in the pressurized chamber in 2008, in collaboration with Dr. Erlend Kristiansen and Prof. Karl Erik Zachariassen, IBI. The experiments in the high pressure tank are divided into two different but integrated parts:

1) Chemical effects of a carbon dioxide leakage at 30 atm pressure.
2) Biological effects of carbon dioxide, pH and trace metals under low and high pressure.

This project has strong relevance also to another global environmental problem; “top-down” Ocean acidification due to increasing atmospheric $CO_2$. Regarding the Ocean Acidification studies we have also cooperation with marine scientist from Analytical and Marine Chemistry Gothenburg University, Sweden, Leibniz Institute of Marine Sciences, IFM-GEOMAR, Kiel, Germany and from Bjerknes Centre for Climate Research, University of Bergen (3)

References:

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*Murat V. Ardelan (previously M. Öztürk)*
*and Eiliv Steinnes*

# Mercury in urine after dental restoration

### These results were presented at a conference. [1]

A major source for human exposure to inorganic mercury is dental amalgam. It has been established that amalgam fillings will slowly release mercury into the oral cavity. For a period of one year one of us (SL) removed 27 amalgam surfaces during 11 sessions in the dentistry. The surfaces were replaced with composite material. Urine samples were collected two hours prior to the dentist appointment and a new sample was collected the next morning. The first 100 ml of urine was discarded and the following 100-150 ml was collected for analyses of creatinin and trace elements. Trace elements were measured using high resolution ICP-MS (Element 2). A decline in urinary mercury level was observed.

### Collection and preparation

### Urine samples

- First morning urine samples were collected in polypropylene vials
- Within two hours samples were divided into two aliquots for creatinin and mercury analysis respectively
- Creatinin samples were kept at -20C until analysis using standard clinical chemistry methods
- Mercury samples were preserved with 0.1 M $HNO_3$

### Hair samples

- Hair samples were cout to a length of approx. 4cm and was further cut into 1 cm sections
- Samples were stored closed containers until further processing
- Prior to analysis the hair samples were washed twice with distilled water and then digested with 50% v/v $HNO_3$ using UltraClave (Milestone) at maximum temperature at 250C. Digested samples were diluted to 0.6M $HNO_3$

### Analytical procedure and quality control

- Samples were analyzed using HR-ICP-MS (Element 2, Bremen, Germany) equipped with Pt cones using low resolution for Hg measurements.
- Multielement standards in 0.1M $HNO_3$ were matrix matched for urine and hair samples respectively
- As reference materials Seronorm and human hair (GBW09101) were used and accuracy was values obtained were within 20% of the specified values.
- Analytical RSD during analysis was below 15% for all measurements

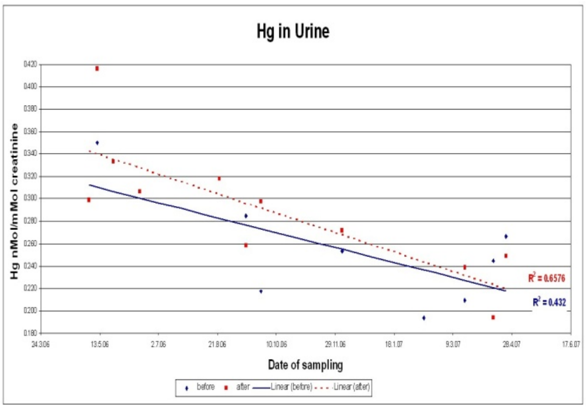
### Comments

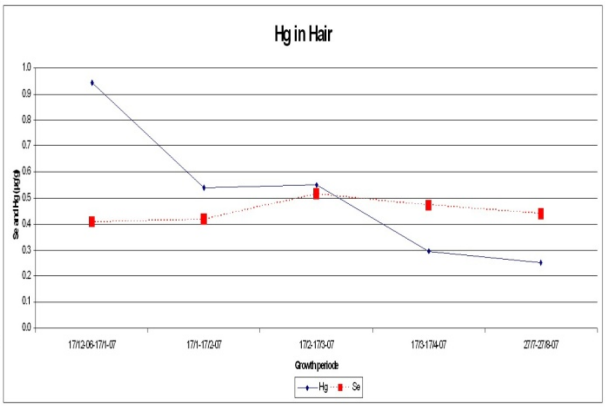
- The reduced mercury levels in urine are confirmed by the hair analysis. Thus we feel confident that the removal of dental amalgam fillings do indeed reduce the mercury body burden
- The urine mercury levels in samples taken after dental work appears to be higher than for samples taken immediately before restoration work. This has been observed also in earlier studies and indicate that the restoration work induce a short term inhalation exposure to the patient.
- The zinc and selenium values obtained in urine indicate no major changes in e.g. dietary habits during the study period.
- For copper there is a decline in urine values for samples taken prior to restoration work during the observation period. However, if we remove sample obtained at 11.05.06 the observed change is cancelled.

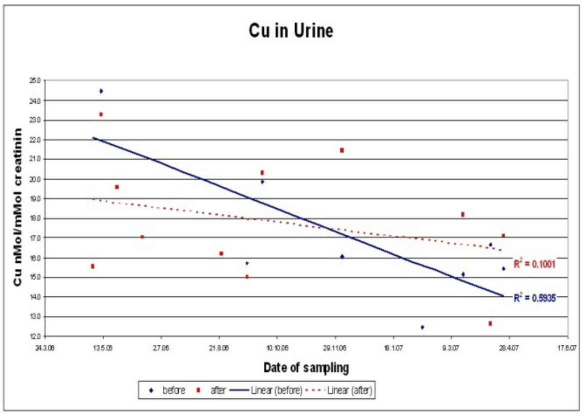
### Dental restoration

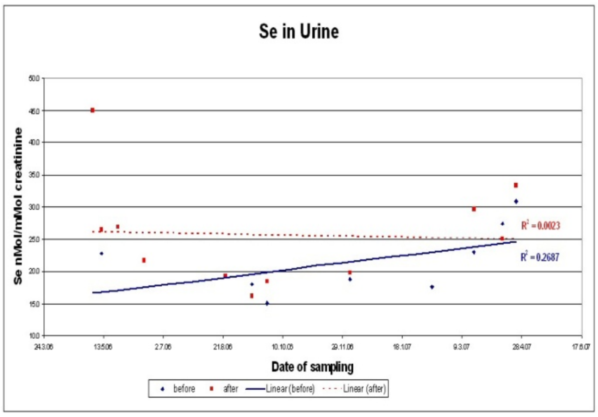
| Date | Surfaces | Pre-sample | Post-sample | Tooth | Remarks |
|---|---|---|---|---|---|
| 04.06.06 | 3 | | * | Molar | |
| 11.05.06 | 1 | * | * | Molar | |
| 25.05.06 | 4 | | * | Molar | |
| 16.06.06 | 2 | | * | Corner | |
| 23.08.06 | 1 | | * | Front | |
| 14.09.06 | 3 | * | * | Corner molar | |
| 28.09.06 | 2 | * | * | Molar | |
| 06.12.06 | 3 | * | * | Corner molar | |
| 12.02.07 | 2 | * | | | Canceled |
| 20.03.07 | 3 | * | * | Molar | |
| 13.04.07 | 4 | * | * | Molar | |
| 23.04.07 | 1 | * | * | Corner | |

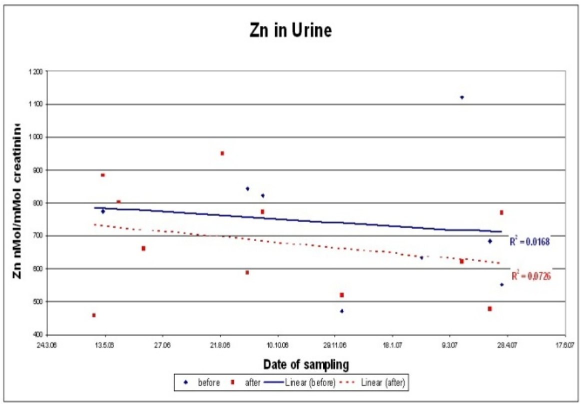
## Illustrations











1. Ref.: International Society For Trace Element Research in Humans (ISTERH) Crete October 21-26 2007. S. Lierhagen, Department of Chemistry; T. Syversen, Department of Neuroscience.

*Syverin Lierhagen*

# Continuous monitoring of heavy metals in groundwater as a tool for the detection and verification of earthquake precursors

Development of an automatic trace metal system has provided an opportunity to monitor earthquake precursor in basaltic rocks. The results clearly indicate changes in the groundwater prior to earthquake, revealing increased electrolabile concentrations of zinc and copper which was possible to monitor with the automatic monitoring station. Maximum values of both pH and electrolabile amounts of zinc and copper was observed 7-8 days before the earthquake. In areas with high earthquake activity new earthquakes can occur at any time - often with severe material damage and even loss of human lives. Development of earthquake warning systems is therefore a highly prioritized research field.

Iceland straddles the mid-Atlantic spreading ridge. Seismic activity occurs at shallow depths and is mainly concentrated to the two transform zones; the South Iceland Seismic Zone and the Tjörnes Fracture Zone. Húsavík is situated close to the Húsavík-Flatey Fault (HHF), which together with the Grimsey Lineament forms the offshore part of the Tjörnes Fracture Zone in northern Iceland.

In September 2006 an automatic system for detecting trace metals was installed at a groundwater source in Iceland, for early warning detection and continuously monitoring. The groundwater samples were analyzed automatically every third hour from the 1st of October 2006. On the 1st of November 2006 at 1:55 pm, a new earthquake of $M_W$ 4.5 on Richter’s scale occurred in Húsavík. Continuous measurements showed significant changes in the electrolabile concentration for several metals 8 days before the earthquake while no metals were visible in the period before that as shown in Figure 1 for zinc and copper. Addition pH was observed to drop, which partly can explain the significant increase the electrolabile metal concentrations in the water. The incidental coincidence of earthquake activity in this area revealed the possible application of such systems for early warning indications of pre-seismic modification of crustal permeability changes which could occur prior to earthquakes.

*Øyvind Mikkelsen, Tonje B. Østebrød, Silje M. Skogvold, Kristina Strasunskiene, Knut. Schrøder, Fredrik Strand*

*Figure1, The monitoring site and system*

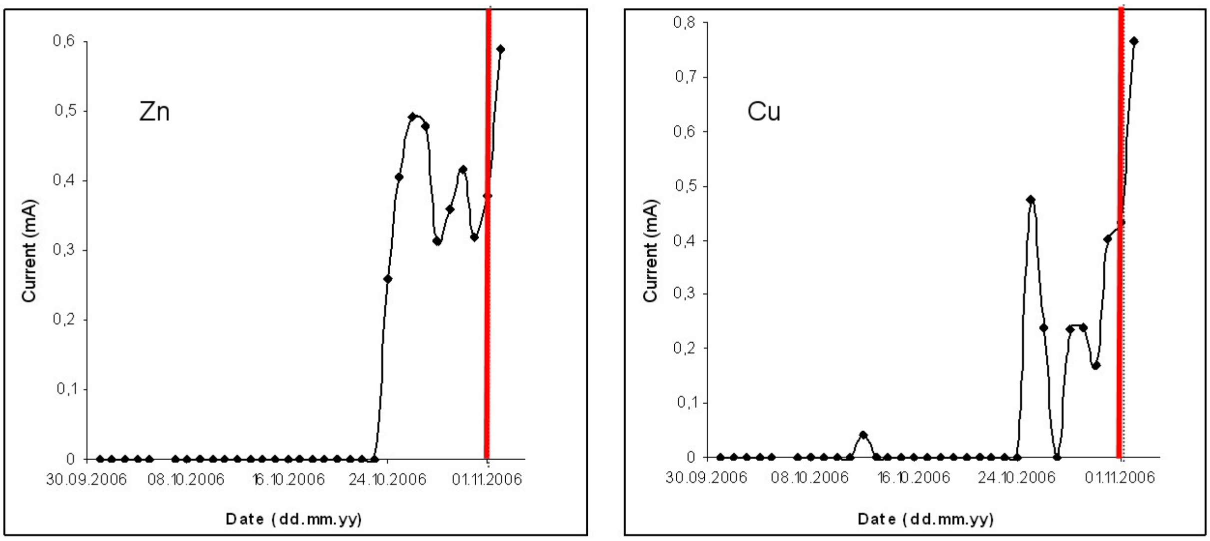


*Figure 2, Average daily current values measured for zinc (left) and copper (right) from October 1$^{st}$ 2006 to November 2$^{nd}$ 2006. The vertical lines (red) indicate the day of the earthquake.*

## Effect of climate change on quantities of NOM and trace metals in water supply sources

This is a collaboration project between our group at Environmental and Analytical Chemistry, Geological Survey of Norway (NGU), Department of Hydraulic and Environmental Engineering (NTNU), Department of Chemistry and Geochemistry Colorado School of Mines, and the Department of Water and Environment at SINTEF. Additionally, two ERASMUS students supervised in our department have been working on this project. The principle objective of this activity is to study the effects of climate change on weathering processes and water quality, including studies on characterisation of natural organic matter (NOM) in surface waters, their variation in time and space, and how their interaction with inorganic weathering processes may vary as a function of changes in climate. This type of study is a prerequisite before making predictions for contents of NOM in drinking water supplies, but also the concentration levels and chemical species of inorganic and synthetic organic potentially toxic contaminants in particular or dissolved form in surface and groundwater. Results from this project will contribute to the understanding of which processes affect water quality in the drainage basin upstream of water supply sources to improve model prediction of future water quality in the wake of climate change. The local or regional characteristics of the e.g. geology, physiography and biology in the ecosystem may modify or enhance various effects of these changes or activities, and has also to be studied.

An interesting aspect in this project is the relationship between the concentrations of trace metals found in river water compared to the concentration found in foam fractions floating on top of the water body. Preliminary results shows significant higher amounts of trace metals in the foam fraction, indicating that the foam fraction acts like a metal collector strongly complexing and binding metals, and through this may be considered an important factor regarding the mobility of trace metals in the environmental. Type of vegetation, strongly linked to the climate, will produce different type of degradation product resulting in different amounts of NOM, and through this in different extent effect the NOM production, the mobility of trace metals, and the water quality.

*Visiting professor Donald Macalady, Department of Chemistry and Geochemistry Colorado School of Mines, sampling foam samples from Jonsvatnet catchment area in Trondheim.*

*Øyvind Mikkelsen*

# XAS (XANES and EXAFS) Investigations of Nanoparticulate Ferrites Synthesized Continuously in Near Critical and Supercritical Water*

The combined electronic and magnetic properties exhibited by ferrite spinels have found applications in catalysis, magnetic media, memory cores, and high-frequency devices. Below a certain dimension, we enter a regime where these properties are affected by crystal or particle size. Over a very wide size range the properties of solid-state materials are constant and seemingly independent of particle size. These bulk, or macroscopic, properties are effectively dominated by the crystal structure from which all of the quantum forces stemming from the constituent atoms are averaged. However, as crystal sizes progressively decrease, a stage is reached below which this averaging is no longer valid. The size-dependent onset of quantum effects is due to the increasing fraction, and hence influences, of surface atoms relative to those within the interior. For most materials, 30-50% of the constituent atoms in 3 nm diameter spherical particles actually lie at the surface. It is around this size limit that surface energy dominates physiochemical properties. Hence, manipulating the dimensions of particles is a central aspect in designing useful materials.

The possibility of designing nanophase ferrites through an environmentally friendly synthetic procedure and, at the same time, fast and continuous was the impetus behind a study on syntheses in near-critical and supercritical water. Heating a fluid toward its critical point causes major changes in its physical properties. In the case of water (critical point: $T_c$ = 374°C; $P_c$ = 218 atm) the transformation is especially significant because it changes from a polar liquid to one that is virtually non-polar and miscible with gases and organic compounds. These changes are spread over a fairly wide temperature range so that around 200°C (near critical) the change in properties is significant enough to make the system synthetically interesting.

*A Fish-eye view of the ring at the European Synchrotron Radiation Facility, Grenoble, France.*

A major reason for interest in the ferrite system stems from varying degrees of flexibility in distributing various cations within the overall spinel $AB_2O_4$ structure (see below). This distribution is mainly a function of the electronic configuration and valence state of the metals within the constraints of the structure, but also the method of preparation and of particle size (>10 nm) can be influential. Thus, depending on the metals, the two types of cation, A and B, frequently exhibit some disordering over two octahedral and one tetrahedral site per formula unit. The temperature dependency of this disorder for a number of spinels with different cation combinations has been extensively discussed in the literature. The cation distribution for a normal spinel can be formally represented by $(A^{2+})_{tet}(2B^{3+})_{oct}(O^{2-})_4$ and for a generalized disordered system by $(A_{1-x}B_x)_{tet}(A_xB_{2-x})_{oct}O_4$, where x is the inversion parameter. For the special case in which x = 1 the spinel is termed "inverse". Included in this study is the ferrite $ZnFe_2O_4$, which is reported to have a normal spinel structure in the bulk phase (no degree of inversion; x = 0), and $Fe_3O_4$, $CoFe_2O_4$, and $NiFe_2O_4$, which in the bulk adopt the completely inverse spinel structure $[(B^{3+})_{tet}(A^{2+}B^{3+})_{oct}(O^{2-})_4]$.

XAS analyses have been used to study the local metal environments in some nanophase ferrites ($Fe_3O_4$, $CoFe_2O_4$, $ZnFe_2O_4$, and $NiFe_2O_4$) prepared by hydrothermal syntheses in near-critical and supercritical water. For the purpose of comparison, a CoFe2O4 sample was hydrothermally synthesised. XANES and EXAFS give useful information about the local metal surroundings in the ferrites. Both regions of the XAS together with calculations of the actual or apparent multiplicities of the different interactions in the model structures have been used to distinguish between the normal and inverse structures. The results of the Scherrer estimation of particle size is questioned because of discrepancies with the EXAFS. This is mainly attributed to the highly polydisperse nature of the products of this method of synthesis since the validity of the Scherrer method is founded on samples being near-monodisperse.

XANES and EXAFS results have shown the following:

(1) The nearest surroundings of iron in nanophase $Fe_3O_4$, compared to the model compound (bulk $Fe_3O_4$), remain unchanged in the nanophase.

(2) Nanophase $CoFe_2O_4$ adopts the inverse spinel structure independent of the synthetic procedure (supercritical water or conventional hydrothermal synthesis). However, the presence of smaller nanoparticles is reflected in the composite metal···metal interactions with lower multiplicities in the nanophase. These results are heavily weighted toward particle sizes around 10 nm in a polydisperse material.

(3) Nanophase $NiFe_2O_4$, synthesized under supercritical conditions at 200ºC and 400ºC, yields products of inverse spinel and metallic nickel. The nickel biproduct is much higher at the lower synthesis temperature.

(4) Nanophase $ZnFe_2O_4$, synthesized under supercritical conditions, consists of a broad range of particles sizes together with some magnetite and iron metal. However, the quality of the data is good enough to establish that zinc ferrite adopts a normal spinel structure under these conditions.

*Nilsen, M.H., Nordhei, C., Ramstad, A.L., Nicholson, D.G., Poliakoff, M., and Cabanas, A. *J. Phys. Chem.* C, 111, 17, 6252, 2007

*Camilla Nordhei*

# Swiss-Norwegian Beamlines: A Unique Combination – Raman spectroscopy Integrated into a Synchrotron Beamline

The Swiss-Norwegian Beamlines (SNBL) at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France are owned and operated by the SNX Foundation. SNX is a consortium of Norwegian(N) and Swiss(CH) universities and funding agencies.

*Administration building ESRF*

In 2007 SNX Council acquired funds to purchase and incorporate a Raman spectrometer into the EXAFS and XRD powder diffraction beamline. The decision to develop the instrumentation was based on successful tests carried out in 2006 at SNBL by groups from Norway, Switzerland and the UK using a loaned spectrometer. This development puts the SNBL at the forefront in being able to carry out simultaneous experiments using the three complementary techniques. The funds were divided 50:50 between the Norwegian and Swiss Research Council. Responsibility for applying to their respective countries was assigned to DavidNicholson (NTNU;Norway) and Jan-DierkGrunwaldt (ETH; Switzerland).

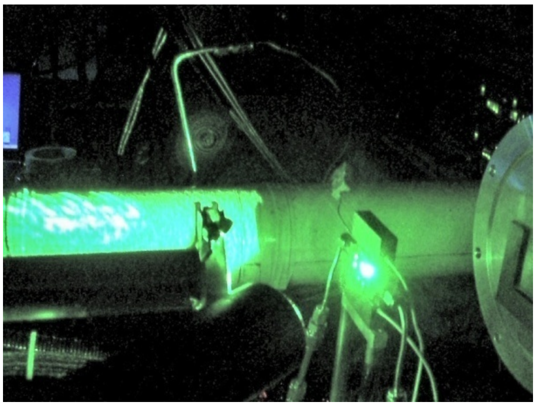
**Pooling of expertise**
The project involves pooling expertise between different Norwegian groups at the Norwegian University of Science and Technology, the University of Oslo and the Institute for Energy Technology and of course with the partnership´s Swiss universities. There is also input from groups outside the SNBL partnership itself but linked scientifically to the SNBL, for example the Royal Institution, UK and Nottingham Trent University.

The international nature of the SNBL project means that the Norwegian and Swiss sides can pool financial as well as human resources to achieve a very cost effective result so that each country gains access to a unique setup for a modest outlay. These pooled resources greatly strengthen the project through the design of various components of instrumentation required for the different experiments.

**Quality of research**
There is no doubt as to the quality of the research carried out at the SNBL. The beamlines have been independently evaluated several times by the ESRF (according to contract) and found the most productive (in terms of publications) of all the beamlines at the ESRF. In effect, the SNBL may be regarded as a national laboratory for each country. The overall Norwegian share of the proposed investment in the integrated Raman system reflects a significant coordination of activities and resources that will satisfy different requirements and will facilitate effective national exploitation of the equipment.

**The Beamline and Raman spectroscopy**
The SNBL comsists of two beamlines and the one we are concerned with here is the unfocused line dedicated to X-ray powder diffraction (XRD) and absorption spectroscopy (XAS). These are the techniques of choice for studying long- and short-range order respectively in the solid state. In contrast, Raman spectroscopy is able to probe the scale between these two extremes. This is what makes the combination interesting to groups in both countries because all three techniques have in common that they are very suitable for *in situ* studies on a wide range of problems relating to various materials e.g. catalyst materials at relevant working conditions. Indeed, the combination is necessary for some studies. For example, the charge/defect distributions that are important properties in some materials are not detectable by XRD

techniques but Raman scattering provides this information.



*EXAFS setup at SNBL illuminated by laser*

The synergy between the synchrotron techniques and Raman spectroscopy is very attractive in advanced studies and a number of combined Raman and XRD or XAS experiments have been performed *ex situ*. However, more complex scientific problems cannot be satisfied by the *ex situ* approach. Fortunately, we are now at a stage where current methodology permits more ambitious experiments in which it is possible to fully integrate the techniques and carry out *in situ* experiments on the same sample under identical conditions.

This integrated approach is only possible at a synchrotron. To the best of our knowledge no current general user facility exists that offers this combination on a routine basis. The SNBL offers its users a truly multipurpose Raman-synchrotron user facility.

*David G. Nicholson*

# Combined X-ray absorption, X-ray powder diffraction and Raman study on cluster formation in zeolites; effect of pore geometry.

Adding hydrogen to the selective catalytic reduction (SCR) hydrocarbons (HC) deNOx process over silver systems leads to enhanced activity. This has been ascribed to the formation of silver nano clusters. Subsequent treatment in NO disperses the metal clusters through oxidation to silver(I). We believe that silver(I) is redispersed to the original protonic sites in within the pores. The reversibility of the valence states with the formation of clusters in both systems is significant part of the overall mechanism for reducing NOx (Fig. 1).

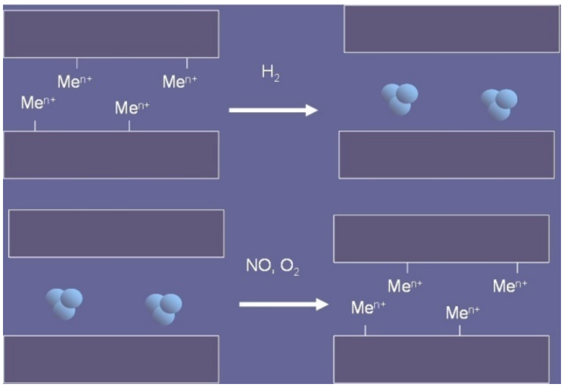


*Fig.1 Proposed mechanism for the reduction of NOx over metal nano clusters.*

The silver environments in the two microporous systems Ag:ZSM-5 and Ag:Y have been studied by in situ X-ray Absorption spectroscopy (XAS) at the Ag K-edge. Samples were heated stepwise in hydrogen while collecting Extended X-ray Absorption Fine Structure (EXAFS), powder diffraction (XRD) and Raman spectroscopy to determine the cluster size as a function of temperature. The EXAFS yields information about the local silver environments such as bond distances and number of neighbours. Silver(I) is reduced by hydrogen to form clusters of metallic silver, but the degree of reduction depends on the parent zeolite. The reduction starts below 100°C for both zeolites and is complete at 350°C. This is seen by the decreased contribution from the Ag-O bond and subsequent formation of an Ag-Ag bond in the Fourier Transform of Ag:Y in Fig. 2.

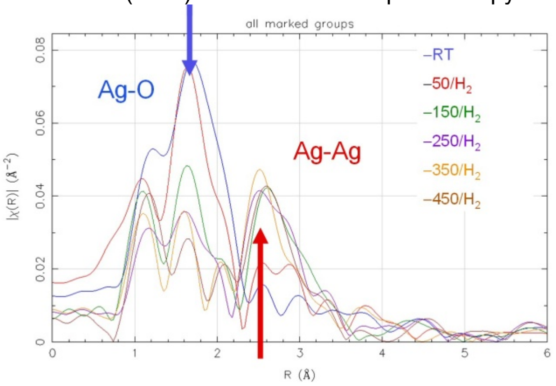


*Fig. 2 Fourier Transforms of ion exchanged Ag:Y heated in hydrogen.*

The coordination numbers of the Ag-Ag neighbouring shell are shown in Fig. 3. Silver metal with its fcc structure has a coordination number of 12 in the bulk form, and coordination numbers of 2-3 are generally expected for nano clusters. It is clear from the EXAFS that nanoclusters are formed in both zeolites at temperatures between 150 and 250°C.

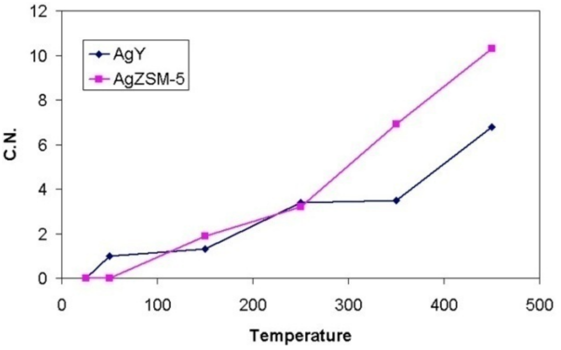


Fig. 3 Coordination number of silver clusters in zeolites Y and ZSM-5 from EXAFS analysis.

The results are consistent with powder diffraction (Fig. 4) which for ZSM-5 contains peaks stemming from silver clusters that appear from 350°C. The size of clusters are 60-100 Å (the shift in position is due to the large thermal expansion coefficient of silver). The silver peak is only barely visible for zeolite Y, and only at the highest temperature of 450°C, thus confirming that cluster size is limited by pore geometry. It is also clear that the nanoclusters formed between 150°C and 250°C are too small to be detected by XRD. The parent material is unaffected by the heating and formation of silver clusters. We believe that small clusters are initially formed inside the pores of both zeolite systems, which then sinter upon further heating. For ZSM-5 the larger clusters are allowed to disperse out of the pores, forming larger nanoclusters on the external surface. This is attributed to the zig-zag structure of ZSM-5 formed by interconnecting 10-rings. In zeolite Y the clusters are trapped in the supercages thus limiting the size of the clusters.

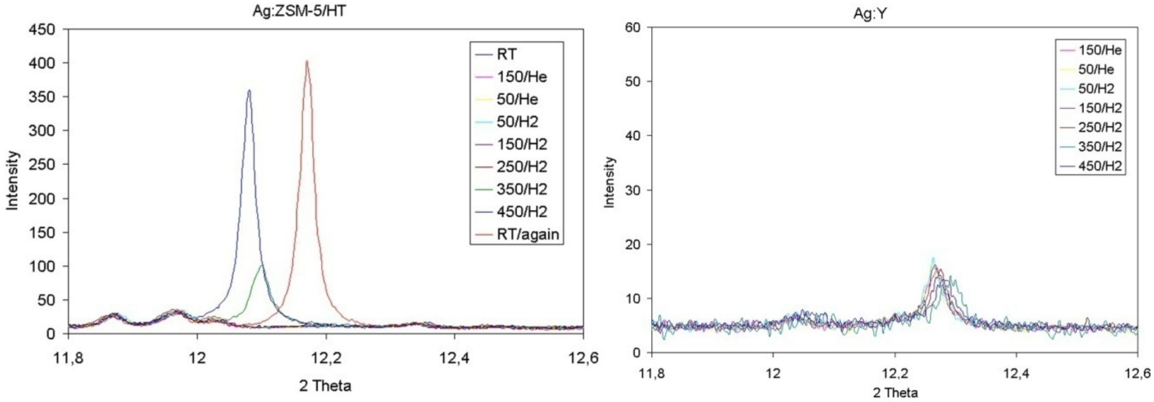


*Fig. 4 Powder diffractograms displaying the (111) reflection of silver appearing during heating in hydrogen for the two zeolite systems.*

This study also included Raman spectroscopy to possibly detect the formation of surface species, or new phases not detectable by XAS or XRD. We encountered several problems with the zeolites materials, the most noticable is the increased background when heating the samples due to fluorescence from the sample (Fig. 5) The Raman spectra of zeolite Y during dehydration in helium by ramping to 150°C clearly shows the peak attributed to the O-H stretching mode at 3700cm$^{-1}$. This arises from water in the system but also protonic sites in the zeolites. The intensity of this peak is clearly reduced during removal of water. The peaks between 1150-1650cm$^{-1}$ are ascribed to vibrational and stretching modes of the zeolite lattice.

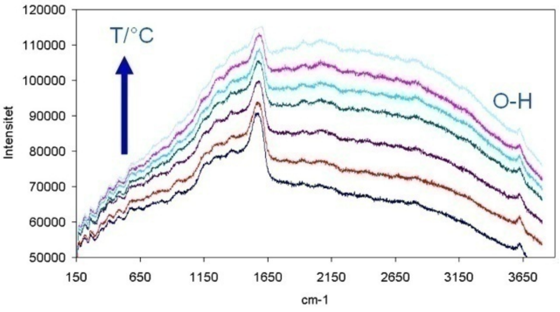
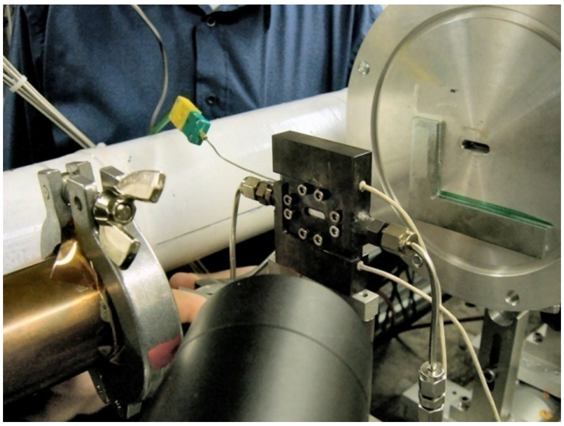


*Fig. 5 Raman spectra of dehydration of Ag:Y to 150°C in helium.*



In situ *cell used for combined experiments on the Swiss Norwegian beamlines, ESRF, Grenoble.*

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*Karina Mathisen*

# Decomposition of carbon dioxide over the putative cubic spinel nanophase cobalt, nickel and zinc ferrites

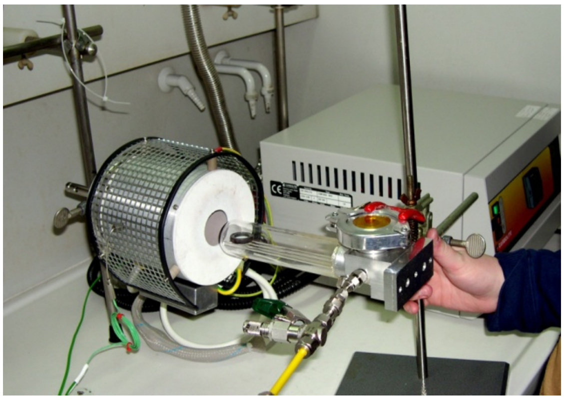
The dynamic alternation between stoichiometry and non-stoichiometry in spinel ferrites ($A(II)Fe(II)_2O_4$) is an important feature that can be exploited in gas reactions. These reactions involve lattice oxygen, either through the transfer of oxygen atoms from the ferrite to the gas (oxidation reaction) or through oxygen vacancies being replenished by oxygen from the gas (reduction reaction). The latter process requires the non-stoichiometric form which can be obtained by the use of a reducing agent such as hydrogen. These non-stoichiometric or oxygen-deficient ferrites can be used to decompose water to hydrogen and carbon dioxide to carbon[1]. We envisage the reaction of ferrites with mixtures of $H_2O$ and $CO_2$ as being especially attractive in this context.

A part of our work[2] on this system is to measure the efficacies of a series of cubic spinel ferrites in abstracting oxygen from carbon dioxide in the absence of water. Oxygen-deficient ferrites are particularly interesting because they exhibit high decomposition efficiencies for both water and carbon dioxide at temperatures as low as 300 °C.

Nanophase (4-6 nm) cobalt, nickel and zinc spinel ferrites were synthesised by coprecipitation and the decomposition of carbon dioxide at 300°C was studied. Oxygen deficiency was obtained by reducing the materials in hydrogen. The divalent metals strongly influence the extent of the reactions; oxygen-deficient nickel ferrite was found to reduce three and nine times more carbon dioxide than the zinc and cobalt analogues, respectively. Carbon monoxide rather than carbon is produced for all of these ferrites.

The reducibility in hydrogen and the degrees of oxygen-deficiencies were studied by X-ray Absorption Spectroscopy at the Swiss-Norwegian Beamline, European Synchrotron Radiation Facility, Grenoble, France. The X-ray Absorption Near Edge Structure reveals that removing oxygen from the spinels leads to the concomitant reduction of iron(III) to iron(II), while the valence state of the divalent metal is unchanged. Of the three ferrites, nickel ferrite exhibits the highest degree of oxygen-deficiency. Extended X-ray Absorption Fine Structure of the nickel ferrite shows that although minor amounts of metallic nickel are expelled through over-reduction, the material is oxygen-deficient in a putative spinel structure.

In the decomposition of carbon dioxide on nanophase oxygen-deficient ferrites, we have shown that their activity and behaviour depend on the divalent A metal. One of the factors governing the reactivities of cobalt, nickel and zinc ferrites is the degree of oxygen-deficiency. This is influenced by the electronic properties of the A metal. Another factor is particle size because within the lower reaches of the nanoregime the degree of non-stoichiometry or oxygen-deficiency is increased relative to the bulk. Significantly, nickel ferrite, which exhibits the largest oxygen-deficiency when reduced in hydrogen, also consumes the largest amount of carbon dioxide. The excellent behaviour of nickel ferrite compared to cobalt and zinc is ascribed to the increased fraction of octahedrally coordinated iron. The degree of oxygen deficiency also affects the reaction mechanism; low oxygen deficiencies appear to favour carbon dioxide reduction to carbon monoxide.



*Reaction cell for EXAFS experiments*

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*Camilla Nordhei and David G. Nicholson*

## Multi-disciplinary chemistry education

In 2007 a multi-disciplinary and multi-lateral NUFU project was awarded to a group consisting of the Chemistry education group at the Department of Chemistry together with the Norwegian Centre for Child Research, the Departments of Geography and Anthropology at NTNU, the University of Zambia and the University of Dilla (Ethiopia). The research project is named “Children, youth and indigenous knowledge in Ethiopia and Zambia” and the main aim is to develop research-based master programs in the South within these fields. In addition to the direct NUFU funding a number of PhD students recruited from the South are associated with the project with financial support from the Norwegian Quota program.

*Illuminated manuscript*

The chemistry education contribution to the project has two main thrusts. One direction of the project is to work within the field of small-scale and low cost chemistry, where we, together with Dilla University, will conduct research on experiments, equipment and the implementation of a practical approach with appropriate technology in schools and undergraduate courses where laboratory facilities are scarce. Although mainly geared to the South, the outcome is also relevant to the Norwegian educational system. The project will not be developing micro-scale equipment which often is too flimsy and difficult to handle and observe. Equipment developed will be smaller than conventional, but will not be allowed to compromise the ability to conduct comprehensive chemistry experiments (in the classroom). Collaboration has been initiated with the North West University of South Africa which is in the forefront within this field.

*Illuminated manuscript*

The second direction is to conduct chemical analysis (e.g. XRF, PIXE, PIGE, XRD, SSIMS) of some pigments of ancient paintings/ illuminated manuscripts in Ethiopian churches and monasteries. This chemical knowledge will be sustained by oral and written sources. The outcome is to benefit conservation and restoration, but an aim is also to rechannel this indigenous knowledge back to the Ethiopian schools, through contextual experiments, as for example the reconstruction of pigments.

*Mural*

*Lise Kvittingen*

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**Ingebrigtsen, Stian; Lundgaard, Lars Esben; Åstrand, Per-Olof.** Effects of additives on prebreakdown phenomena in liquid cyclohexane: II. Streamer propagation. *Journal of Physics D: Applied Physics* 2007; 40(18): 5624-5634

**Inzoli, Isabella; Simon, Jean-Marc; Kjelstrup, Signe; Bedeaux, Dick.** Thermal effects during adsorption of n-butane on a silicalite-1 membrane: A non-equilibrium molecular dynamics study. *Journal of Colloid and Interface Science* 2007; 313: 1-11

*Students at work*

**Johannessen, Eivind; Bedeaux, Dick.** Integral Relations for the Interfacial Heat and Mass Transfer Resistivities and the Inverted Temperature Profile. *Physics of fluids* 2007; 19: 017104, 1-7

**Johannessen, Eivind; Røsjorde, Audun.** Equipartition of entropy production as an approximation to the state of minimum entropy production in diabatic distillation. *Energy* 2007; 32(4): 467-473

**Kjelstrup, Signe; Bedeaux, Dick.** Heat and mass transfer across phase boundaries: Estimates of coupling coefficients. *Atti dell´Accademia Peloritana dei Pericolanti Classe di Scienze Fisiche, Matematiche e Naturali* 2007; 85

**Kjelstrup, Signe; Hustad, Johan Einar; Gundersen, Truls; Lior, Noam.** 18th International conference on efficiency, costs, optimization, simulation, and environmental impact of energy systems - Trondheim, Norway, June 22-24, 2005 - Introduction. *Energy* 2007; 32(4): 247-248

**Koper, Ger J.M. ; Kjelstrup, Signe; van de Ven, Theo; Sadeghi, Moshen; Douglas, W.J.M.** Entropy production for cylinder drying of linerboard and newsprint. *International Journal of Heat and Mass Transfer* 2007; 50: 1344-1355

**Mathisen, Karina; Nicholson, David Graham; Beale, AM; Sanchez-Sanchez, M; Sankar, G; Bras, W; Nikitenko, S.** Comparing CuAPO-5 with Cu:ZSM-5 in the Selective Catalytic Reduction of NOx: An in situ Study. *Journal of Physical Chemistry C* 2007; 111(7): 3130-3138

**Meland, Anne-Kristine; Kjelstrup, Signe.** Three steps in the anode reaction of the polymer electrolyte membrane fuel cell. Effect of CO. *Journal of electroanalytical chemistry and interfacial electrochemistry* 2007; 610(2): 171-178

**Nilsen, Merete Hellner; Antonakou, Eleni; Bouzga, Aud; Lappas, Angelos; Mathisen, Karina; Stöcker, Michael.** Investigation of the effect of metal sites in Me-Al-MCM-41 (Me=Fe, Cu or Zn) on the catalytic behavior during the pyrolysis of wooden based biomass. *Microporous and Mesoporous Materials* 2007; 105: 189-203

**Ortiz de Zárate, José; Sengers, J.V.; Bedeaux, Dick; Kjelstrup, Signe.** Concentration fluctuations in nonisothermal reaction-diffusion systems. *Journal of Chemical Physics* 2007; 127

**Ratushnaya, Valeria; Bedeaux, Dick; Kulinskii, Vladimir; Zvelindovsky, Andrei.** Stability properties of the collective stationary motion of self-propelling particles with conservative kinematic constraints. *Journal of Physics A: Mathematical and Theoretical* 2007; 40: 2573-2581

**Rubi, Miguel; Bedeaux, Dick; Kjelstrup, Signe.** Unifying thermodynamic and kinetic descriptions of single-molecule processes: RNA unfolding under tension. *Journal of Physical Chemistry. B, Condensed Matter, Materials, Surfaces, Interfaces & Biophysical* 2007; 111: 9598-9602

**Rubi, Miguel; Naspreda, Manel; Kjelstrup, Signe; Bedeaux, Dick.** Energy Transduction in Biological Systems: A Mesoscopic Non-Equilibrium Thermodynamics Perspective. *Journal of Non-Equilibrium Thermodynamics* 2007; 32: 351-378

**Røsjorde, Audun; Kjelstrup, Signe; Johannessen, Eivind; Hansen, Roger.** Minimizing the entropy production in a chemical process for dehydrogenation of propane. *Energy* 2007; 32(4): 335-343

**Shen, Quang; Brown, J. W.; Richardson, A. D.; Hagen, Kolbjørn.** The molecular structure and conformation of trichloronitromethane as determined by gas-phase electron diffraction and theoretical calculations. *Journal of Molecular Structure* 2007; 830: 204-207

**Simon, Jean-Marc; Inzoli, Isabella; Bedeaux, Dick; Kjelstrup, Signe.** Numerical evidence for a thermal driving force during adsorption of butane in silicalite. *Molecular Simulation* 2007; 33: 839-841

**Stølevik, Reidar Edvald**. Diamanter. *Kjemi* 2007(5): 16-18

**Svelle, Stian; Olsbye, Unni; Joensen, Finn; Bjørgen, Morten.** Conversion of methanol to alkenes over medium and large pore acidic zeolites: Steric manipulation of the reaction intermediates governs the ethene/propene product selectivity. *Journal of Physical Chemistry C* 2007; 49(111): 17981-17984

*Old Trondheim, Bakklandet*

**Xu, Jing; Kjelstrup, Signe; Bedeaux, Dick; Simon, Jean-Marc.** The heat of transfer in a chemical reaction at equilibrium. *Journal of Non-Equilibrium Thermodynamics* 2007; 32(3): 341-349

**Xu, Jing; Kjelstrup, Signe; Bedeaux, Dick; Simon, Jean-Marc.** Transport properties of 2F = F_2 in a temperature gradient as studied by molecular dynamics simulations. *Physical Chemistry, Chemical Physics* 2007; 9: 969-981

**Yamaki, Daisuke; Koch, Henrik; Ten-no, Seiichiro.** Basis set limits of the second order Møller-Plesset correlation energies of water, methane, acetylene, ethylene and bezene. *Journal of Chemical Physics* 2007; 127(14): 144104-144108

**Zvolinschi, Anita; Kjelstrup, Signe; Bolland, Olav; van der Kooi, Hedzer.** Exergy sustainability indicators as a tool in industrial ecology. Application to two gas-fired combined cycle power plants. *Journal of Industrial Ecology* 2007; 11(4): 85-98

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

**B. Alsberg**

Research Co-operation at University of Bergen, Norway, May 22 – 25, 2007.

Conference NIR 2007, Umeå, Sweden, June 15 – 21, 2007.
Lecture on: A Hyperspectral Projection System.

Lecture and Meetings with Collaborating Partners in Aberystwyth, Wales and UMIST, Manchester, UK, Sep. 3 – 7, 2007.

Industrial Visit to ChemSpeed, Basel, Switzerland, Oct. 30 – Nov. 1, 2007.

Interview in Gemini: Gjør det usynlige synlig. Dec. 1, 2007.

Interview in Dagbladet: Nytt kamera ser alt. Dec. 3, 2007.

Interview in Universitetsavisa: Gjør det usynlige synlig. Dec. 5. 2007.

**T. Andreassen**

Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentation: Stereoselective Enereactions with N-sulfinyl Sulfinamides”.

Bruker Biospin’s pre-ENC Meeting/Workshop, Daytona Beach, Florida, USA, April 20 – 21, 2007.

48th ENC (Experimental Nuclear Magnetic Resonance Conference), Daytona Beach, Florida, USA, April 22 – 27, 2007.

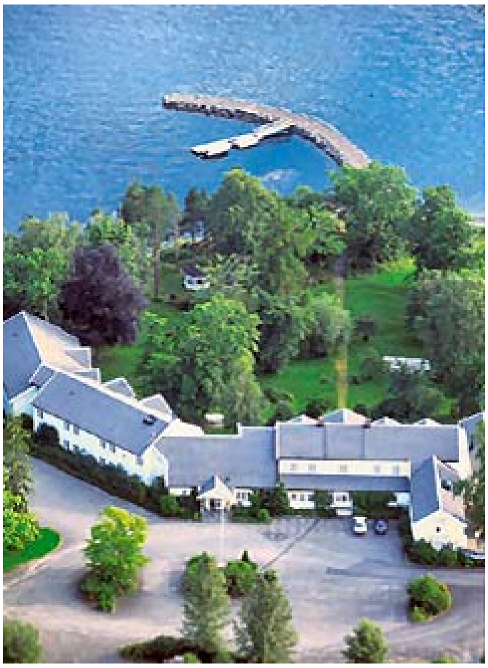
**T. Anthonsen**

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.

Workshop “Applied Biocatalysis COST Action D25”, Røros, Norway, Jan.13, 2007.

Co-organizer of the Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Lecture on: Studies of Charge Delocalized Cations Prepared by Reaction with Deuterated Trityl Cation.



*Jægtvolden Fjordhotell, Inderøy*

Co-author on Poster Presentations: “Studies of the Catalytic Centre of Lipase A from Candida Antarctice”, “Studies of Charge Delocalized Cations Prepared by Reaction with Deuterated Trityl Cation”, “Chemo-enzymatic Synthesis of Iminocyclitols. Potential Inhibitors of Glycosidases and Glycosyl Transferases, “Chemo-enzymatic Methods for Synthesis of Enantiopure Biologically Active Compounds”, “Chemo-enzymatic Synthesis of Chiral Building Blocks Based on Para-Hydroxpropiophene”, “Chemo-enzymatic Synthesis of Chiral Building Blocks Based on Para-Hydroxpropionphene”, “Chemo-enzymatic Synthesis of Enantiopure □-Alkyl-□, □-Dihydroxy Units” and “Chemo-enzymatic Synthesis of Enantiopure Alpha-Alkyl-Alpha,Beta-Dihydroxy Units”.

Research Co-operation at Alexandria University, Egypt, Feb. 26 – March 2, 2007.
Guest Lecture: Biocatalysis in Organic Chemical Synthesis, Feb. 26, 2007.

Chairman for “COST D25 Training School in Biocatalysis”, Certosa de Pontignano, Siena, Italy, April 27 – May 4, 2007.
Opening Remarks and Information about: EU FP7 CALLS in Biocatalysis.

Conference “Organisk kjemisk høstmøte”, Oslo, Norway, Oct. 19, 2007.

Roger Sheldon Symposium: ”Green Chemistry and Biocatalysis”, TU Delft, Netherlands, Dec. 6 – 7, 2007.

**F.G. Banica**

19th International Symposium on Bioelectrochemistry and Bioenergetics, Toulouse, France, April 1 – 4, 2007.
Co-author on Poster Presentations: "Seleno-Methionine in Adsorbed State at Electrified Metal Surfaces" and "Electrochemical Reactivity of Homocysteine (Hcy) at a Mercury Electrode in the Presence of Nickel Ion".

Conference "EuroAnalysis XIV", Antwerp, Belgium, Sep. 9 – 14, 2007.
Co-author on Poster Presentations: "Homocysteine Electrochemical Reactions at a Mercury Electrode in the Presence of Nickel or Cobalt Ions" and "Electroanalytical Chemistry of Metal Sulfides at Mercury Electrodes: Thiourea as a Starting Material for Metal Sulfide Preparation".

**D. Bedeaux**

Leave of Absence Aug. 1 – Dec. 31, 2007

Research Stay at Centre for Advanced Study, Oslo, Norway, Aug. 1 – Dec. 31, 2007.

Seminar at Imperial College, London, UK, Feb. 7 – 8, 2007.
Co-author on Lecture on: Heat and Mass Transfer into and through Interfaces.

Visit at ETH, Zürich, Switzerland, May 2 – 11, 2007.
Guest Lecture on: Heat and Mass Transfer into and through Interfaces.

Joint European Thermodynamics Conference IX, St. Etienne, France, June 12 – 15, 2007.
Co-author on Lecture on: Transport Properties of a Reacting Mixture in a Temperature Gradient as Studied by Molecular Dynamics Simulations.

10th UK Heat Transfer Conference, Edinburgh, UK, Sep. 10 – 11, 2007.
Co-author on Lecture on: Surface Transfer Coefficients in Non-Equilibrium Thermodynamics Studied by Non-Equilibrium Molecular Dynamics Simulations.

Conference "Thermodynamics 2007", Paris, France, Sep. 26 – 28, 2007.
Co-author on Lecture on: Non-Isothermal Adsorption of N-Butane on Silicalite by Transient Non-Equilibrium Molecular Dynamics Simulation.
Co-author on Poster Presentations: "Transfer Coefficients for Evaporation of a System with a Lennard-Jones Long Range Spline Potential" and "Transport Properties of a Reacting Binary Fluid, A Non-Equilibrium Molecular Dynamics Simulations Study".

Meeting the Entropy Challenge. An International Symposium in Honor and Memory of Professor Joseph Henry Keenan, MIT, Cambridge, Mass., USA, Oct. 4 – 5, 2007.
Lecture on: The Second Law of Thermodynamics and Statistical Mechanics.

Seminar at the Centre for Advanced Study, Oslo, Norway, Oct. 18, 2007.
Guest Lecture on: Muscular Contraction and the Calcium Pump.

*Skarnsund bridge, Inderøy*

**T. Berg**

European Research Course on Atmospheres, Grenoble, France, Jan. 8 – Feb. 11, 2007.
Co-author on Lecture on: Mercury in the Arctic.

20th Task Force Meeting on the UNECE ICP Vegetation, Dubna, Russia, March 5 – 9, 2007.
Co-author on Lecture on: 30 Years of Atmospheric Deposition Studies in Norway Using Moss Analysis.

Field Work, Ny-Ålesund, Spitzbergen, April 18 – 27, June 18 – 28 and Aug. 15 – 30, 2007.

Researcher's Night, NTNU, Trondheim, Sep. 28, 2007.
Co-author on Lecture on: Kvikksølv i Arktis.

Workshop "AMAP 2011 Mercury Assessment", Copenhagen, Denmark, Oct. 29 – 31, 2007.
Co-author on Lectures on: "AMDE Activities at Ny-Ålesund, Andøya and Troll" and "COPOL: Contaminants in Polar Regions".

Miljøovervåking, Høgskolen i Troms, Tromsø, Norway, Nov. 15, 2007.
Lectures on: "Luftforurensninger" and "Effekter av luftforurensninger".

Miljøovervåking, Høgskolen i Troms, Tromsø, Norway, Nov. 16, 2007.
Lectures on: ”Klimaendringer og ozonlaget”, ”Tidstrender for luftforurensninger” and ”Utslipp av forurensninger”.

*Strategy seminar at Jægtvolden, Inderøy*

**M. Bjørgen**

Research Co-operation at University of Oslo, Norway, Sep. 10 – 14 and Dec. 18 – 21, 2007.

The 8th Natural Gas Conversion Symposium, Natal, Brazil, May 27 – 31, 2007.
Co-author on Lecture on: Conversion of Methanol to Hydrocarbons: Hints to Rational Catalyst Design from Fundamental Mechanistic Studies on H-ZSM-5.

Conference “EuropaCat VIII”, Åbo/Turku, Finland, Aug. 26 – 31, 2007.
Co-author on Lectures on: “Conversion of Methanol to Hydrocarbons over Medium and Large Pore Acidic Zeolites: Steric Control of the Reaction Intermediates Determines the Ethene/Propene Selectivity”, “Conversion of Methanol to Hydrocarbons: Spectroscopic Characterization of Carbonaceous Species Formed over HZSM-5” and “The Inconsistency in Measured and Expected Adsorption Properties of Metal Organic Frameworks, Exemplified by MOF-5”.
Co-author on Poster Presentation: Thermally Stable Pt/Y-Based Metal-Organic Framework: Exploring the Accessibility and Electronic Properties of the Metal Centers”.

SPECTROCAT International Summer School on Vibrational Spectroscopy, Caen, France, Sep. 16 – 21, 2007.

T. Bruvoll

International Supercomputer Conference 2007, Dresden, Germany, June 25 – 29, 2007.

Conference “Microsoft TechEd”, Barcelona, Spain, Nov. 12 – 16, 2007.

**O. Burheim**

Conference “Hydrogen & Fuel Cells 2007”, Vancouver, BC, Canada, April 29 – May 2, 2007.
Co-author on Lecture on: Through-Plane Thermal Conductivity of Nafion.

**P.H. Carlsen**

Member of The European COST-D31 Committee.

Establishing of Socrates/Erasmus-NTNU Collaboration Agreements with Institute of Chemical Technology, Prague, Czech Rep., University of Perugia, Italy and University of Vienna, Austria.

Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 14, 2007.

**P. – O. Eggen**

Conference “19th Century Chemistry: Spaces and Collections”, Lisbon, Portugal, Feb. 1 – 4, 2007.
Co-author on Lecture on: Yesterday’s Collections in Today’s Courses.

Co-operation Project in Chemistry Didactics at North-West University, Potchefstroom and University of Cape Town, South Africa, Feb. 19 – 27, 2007.

**A. Fiksdahl**

Section Leader, Organic Chemistry Group, Department of Chemistry, NTNU.

Established Co-operation with University of Hamburg, Germany, on NFR-Project.

Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentations: “Synthesis of new β–Carboline Analogues” and “Oxidative Cyclisation of N-Arylaminopyridines”.

8th Annual Florida Heterocyclic IUPAC-Sponsored Conference, Gainesville, Florida, USA, March 11 - 14, 2007.
Co-author on Poster Presentation: Synthetic Applications of β-Pyridylmalonates.

21st International Congress on Heterocyclic Chemistry, University of New South Wales, Sydney, Australia, July 15 – 21, 2007.
Co-author on Poster Presentation on: Synthesis of new β–Carboline Analogues.

**T.P. Flaten**

Deputy Head of the Department of Chemistry.

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

Editor, Norsk Epidemiologi (Norwegian Journal of Epidemiology).

Workshop “TraceSpec 2007”, Münster, Germany, Sep. 4 – 7, 2007.
Co-author on Poster Presentation: High Resolution ICP-MS Trace Element Analysis of Proteins Obtained from Size Exclusion High Pressure Chromatography of Human Cerebrospinal Fluid.

ISTERH Conference on Trace Elements in Diet, Nutrition & Health: Essentiality and Toxicity, Crete, Greece, Oct. 21 – 26, 2007.
Co-author on Lectures on: “Iron and Copper Toxicity in Hereditary Diseases” and “Separation of Proteins in Cerebrospinal Fluid by Size Exclusion HPLC and Determination of Trace Elements by HR-ICP-MS”.
Co-author on Poster Presentations: “A Nation-Wide Survey of Trace Elements in Lynx, Wolverines, Wolves and Brown Bears in Norway”, “Effects of Formalin Fixation on Trace Element Concentrations in Biological Tissue”, “Trace Elements in Cerebrospinal Fluid and Blood from Patients with a Rare Progressive Central and Peripheral Demyelinating Disease” and “Trace Elements in Serum from Patients with Parkinson’s Disease – a Prospective Case-Control Study”.

*Strategy seminar at Jægtvolden, Inderøy*

**E. Fuglseth**

Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentation: Substrate Limitations to the Use of Tetrabutylammonium Hydrogen Difluoride in Nucleophilic Displacements of 2-Bromoacetophenones.

**O.R. Gautun**

Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentations: “Aziridines from L-Aspartic Acid – Synthesis and Ring Opening Reactions” and “Stereoselective Ene-Reactions with N-Sulfinyl Sulfinamides”.

**J. Ge**

Conference “Thermodynamics 2007”, Paris, France, Sep. 26 – 28, 2007.
Co-author on Poster Presentation: Transfer Coefficients for Evaporation of a System with a Lennard-Jones Long Range Spline Potential.

**K. Gellein**

Workshop “TraceSpec 2007”, Münster, Germany, Sep. 4 – 7, 2007.
Co-author on Poster Presentation: High Resolution ICP-MS Trace Element Analysis of Proteins Obtained from Size Exclusion High Pressure Chromatography of Human Cerebrospinal Fluid.

ISTERH Conference on Trace Elements in Diet, Nutrition & Health: Essentiality and Toxicity, Crete, Greece, Oct. 21 – 26, 2007.
Co-author on Lectures on: “Separation of Proteins in Cerebrospinal Fluid by Size Exclusion HPLC and Determination of Trace Elements by HR-ICP-MS” and ”Iron and Copper Toxicity in Hereditary Diseases”.
Co-author on Poster Presentations: “Effects of Formalin Fixation on Trace Element Concentrations in Biological Tissue”, “Trace Elements in Cerebrospinal Fluid and Blood from Patients with a Rare Progressive Central and Peripheral Demyelinating Disease” and “Trace Elements in Serum from Patients with Parkinson’s Disease – a Prospective Case-control Study”.

**O. – E. Haas**

Research Stay at Université de Bourgogne, Dijon, France, Jan. 14 – Feb. 2, 2007.

Research Stay at Centre d’Etudes de Saclay, Saclay, France, May 14 – 31, 2007.

Conference NANOMAT 2007, Bergen, Norway, June 6 – 7, 2007.
Co-author on Poster Presentation: Surface self Diffusion of Hydrogen on Carbon Support.

Conference “Diffusion Fundamentals II”, L`Aquila, Italy, Aug. 25 – 30, 2007.
Co-author on Poster Presentations: “Surface sSelf Diffusion of Hydrogen on Carbon Support by Quasielastic Neutron Scattering”, “Dynamical Behaviour of H2 on Graphite Surface. A Molecular Dynamics Study” and “Dynamical Behaviour of H2 Molecules on Graphite Surface. A Molecular Dynamics Study”.

Research Stay at Institut National Polytechnique de Grenoble, France, Nov. 18 – 27, 2007.

**K. Hagen**

12th European Symposium on Gas Elctron Diffraction, Blaubeuren, Germany, June 24 – 28, 2007.
Co-author on Poster Presentation: N,N-Dimethylthioformamide and N,N-Dimethylthiocaebamoylchloride. Molecular Structure by Gas-phase Electron Diffraction and ab Initio Molecular Orbital- and Density Functional Theory Calculations.

*Strategy seminar at Jægtvolden, Inderøy*

**B.H. Hoff**

Conference "22. Organisk kjemisk vintermøte", Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentations: "Substrate Limitations to the Use of Tetrabutylammonium Hydrogen Difluoride in Nucleophilic Displacements of 2-Bromoacetophenones" and "Chemo-enzymatic Synthesis of Chiral Building Blocks Based on Para-Hydroxpropionphene".

**S. Ingebrigtsen**

28th International Conference on Phenomena in Ionized Gases, Prague, Czech Rep., July 15 – 20, 2007.
Co-author on Poster Presentations: "Spectral Analysis of the Light emitted from Streamers in chlorinated Liquids" and "Spectral Analysis of the Light emitted from Streamers in Liquid CCl4".

**I. Inzoli**

Conference "FOA9", Taormina, Italy, May 20 – 25, 2007.
Co-author on Poster Presentation: Temperature Effects During Adsorption of N-Butane on Silicalite.

Conference "Diffusion Fundamentals II", L`Aquila, Italy, Aug. 25 – 30, 2007.
Co-author on Poster Presentation: Surface Resistance to Heat and Mass Transfer in a Silicalite Membrane. A Non-Equilibrium Molecular Dynamics Study.

Conference "Thermodynamics 2007", Paris, France, Sep. 26 – 28, 2007.
Co-author on Lecture on: Non-Isothermal Adsorption of N-Butane on Silicalite by Transient Non-Equilibrium Molecular Dynamics Simulation.

**E.E. Jacobsen**

Co-organizer of the Conference "22. Organisk kjemisk vintermøte", Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentations: "Stereoselective Enereactions with N-Sulfinyl Sulfinamides", "Chemo-enzymatic Methods for Synthesis of Enantiopure Biologically Active Compounds" and "Studies of the Catalytic Centre of Lipase A from Candida Antarctica".

Interview in Under Dusken: Kjemikerne frifinner benzen. Feb. 13, 2007.

Interview in Adresseavisen: Kjemiker avviser kreft fra benzen. Feb. 14, 2007.

"COST D25 Training School in Biocatalysis", Certosa de Pontignano, Siena, Italy, April 28 – May 3, 2007.
Lecture on: Important Small Molecules. Enantiopure Building Blocks for Biologically Active Compounds.

**S.L. Jensen**

Conference "22. Organisk kjemisk vintermøte", Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Lecture on: Studies of Charge Delocalized Cations Prepared by Reaction with Deuterated Trityl Cation.

**G. Kildahl-Andersen**

Conference "22. Organisk kjemisk vintermøte", Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Lecture on: Studies of Charge Delocalized Cations Prepared by Reaction with Deuterated Trityl Cation.
Co-author on Poster Presentation: Chemo-enzymatic Methods for Synthesis of Enantiopure Biologically Active Compounds.

The 21st International Symposium for Polycyclic Aromatic Compounds, Trondheim, Norway, Aug. 5 – 10, 2007.
Co-author on Poster Presentation: A novel Aromatic Compound in Coal Extracts.

23rd International Organic Geochemistry Meeting, Torquay, Devon, UK, Sep. 9 – 14, 2007.
Co-author on Poster Presentation: Identification of an Early-Eluting Rearranged Hopane Series. Synthesis from Hop-17(21)-Enes and Detection of Intermediates in Sediments.

**S. Kjelstrup**

Professor in part time position at TU Delft, Netherlands, Jan. 2 – Feb. 1 and June 1 – July 1, 2007.

Leave of Absence Aug. 1 – Dec. 31, 2007

Research Stay at Centre for Advanced Study, Oslo, Norway, Aug. 1 – Dec. 31, 2007.

Seminar at Imperial College, London, UK, Feb. 7 – 8, 2007.
Co-author on Lecture on: Heat and Mass Transfer into and through Interfaces.

Conference “Hydrogen & Fuel Cells 2007”, Vancouver, BC, Canada, April 29 – May 2, 2007.
Co-author on Lecture on: Through-Plane Thermal Conductivity of Nafion.

Visit at ETH, Zürich, Switzerland, May 2 – 11, 2007.
Guest Lecture on: Heat and Mass Transfer into and through Interfaces.

Conference “FOA9”, Taormina, Italy, May 20 – 25, 2007.
Co-author on Poster Presentation: Temperature Effects during Adsorption of N-Butane on Silicalite.

Conference NANOMAT 2007, Bergen, Norway, June 6 – 7, 2007.
Co-author on Poster Presentation: Surface Self Diffusion of Hydrogen on Carbon Support.

Joint European Thermodynamics Conference IX, St. Etienne, France, June 12 – 15, 2007.
Co-author on Lecture on: Transport Properties of a Reacting Mixture in a Temperature Gradient as Studied by Molecular Dynamics Simulations.

Conference “Diffusion Fundamentals II”, L`Aquila, Italy, Aug. 25 – 30, 2007.
Co-author on Poster Presentations: “Surface Self Diffusion of Hydrogen on Carbon Support by Quasielastic Neutron Scattering”, “Dynamical Behaviour of H2 on Graphite Surface. A Molecular Dynamics Study”, “Surface Resistance to Heat and Mass Transfer in a Silicalite Membrane. A Non-Equilibrium Molecular Dynamics Study” and “Dynamical Behaviour of H2 Molecules on Graphite Surface. A molecular Dynamics Study”.

10th UK Heat Transfer Conference, Edinburgh, UK, Sep. 10 – 11, 2007.
Co-author on Lecture on: Surface Transfer Coefficients in Non-Equilibrium Thermodynamics Studied by Non-Equilibrium Molecular Dynamics Simulations.

Conference “Thermodynamics 2007”, Paris, France, Sep. 26 – 28, 2007.
Co-author on Lecture on: Non-Isothermal Adsorption of N-Butane on Silicalite by Transient Non-Equilibrium Molecular Dynamics Simulation.
Co-author on Poster Presentations: “Transfer Coefficients for Evaporation of a System with a Lennard-Jones Long Range Spline Potential” and “Transport Properties of a Reacting Binary Fluid, A Non-Equilibrium Molecular Dynamics Simulations Study”.

Article in Magazine at the Centre for Advanced Study, Oslo: Chemists inspired by Nature, Oct. 2, 2007.

Meeting the Entropy Challenge. An International Symposium in Honor and Memory of Professor Joseph Henry Keenan, MIT, Cambridge, Mass., USA, Oct. 4 – 5, 2007.
Lecture on: Frontiers of the Second Law: Can Activated Processes be Described by Non-eEquilibrium Thermodynamics?

**H. Koch**

Leave of Absence Aug. 1 – Dec. 31, 2007.

Research Stay at Centre for Advanced Study, Oslo, Norway, Aug. 1 – Dec. 31, 2007.

Research Project at Universidad de Alicante, Spain, March 3 – 27, 2007.

Research Project at Universidad de Valencia, Spain, April 3 – 12, May 29 – June 27, June 30 – July 13, Aug. 4 – 12, Aug. 25 – 28, Sep. 26 – Oct. 10, Nov. 17 – 26, Dec. 21 – 31, 2007.

Research Project at University of Nagoya, Japan, April 28 – May 17, July 13 – Aug. 4, Oct. 14 – Nov. 8 and Dec. 4 – 18, 2007.

Workshop on “Highly Accurate Calculations of Molecular Electronic Structure”, University of Karlsruhe, Germany, March 24, 2007.
Lecture on: Method Spesific Cholesky Decomposition.

*Strategy seminar at Jægtvolden, Inderøy*

**L. Kvittingen**

Leave of Absence August 1 – Dec. 31, 2007.

Conference “19th Century Chemistry: Spaces and Collections”, Lisbon, Portugal, Feb. 1 – 4, 2007.
Co-author on Lecture on: Yesterday’s Collections in Today’s Courses.

Co-operation Project in Chemistry Didactics at North-West University, Potchefstroom and University of Cape Town, South Africa, Feb. 19 – 27, 2007.

Research Project at University of Oslo, Norway, April 23 – May 3, 2007.

In-Service Chemistry Workshop, North-West University, Potchefstroom, South Africa, Oct. 2 – 4, 2007.
Lecture on: Small Scale Chemistry.

Research Stay at North-West University, South Africa, Oct. 11 – Nov. 14 and Nov. 28 – Dec. 31, 2007.

In-Service Teacher Training Workshop, North-West University, Britts, South Africa, Oct. 13 – 14, 2007.
Lecture on: Small Scale Electrochemistry.

In-Service Teacher Training Workshop, North-West University, Wryberg, South Africa, Oct. 19 – 21, 2007.
Lecture on: Small Scale Electrochemistry.

Research Stay at Dilla College of Health Sciences, Dilla, Ethiopia, Nov. 14 – 28, 2007.

**S. Lierhagen**

ISTERH Conference on Trace Elements in Diet, Nutrition & Health, Crete, Greece, Oct. 21 – 26, 2007.
Co-author on Poster Presentations: “A Nation-Wide Survey of Trace Elements in Lynx, Wolverines, Wolves and Brown Bears in Norway”, “Trace Elements in Cerebrospinal Fluid and Blood from Patients with a Rare Progressive Central and Peripheral Demyelinating Disease”, “Trace Elements in Serum from Patients with Parkinson’s Disease – a Prospective Case-Control Study” and “Mercury in Urine after Dental Restoration”.

**A. Lykknes**

Conference “19th Century Chemistry: Spaces and Collections”, Lisbon, Portugal, Feb. 1 – 4, 2007.
Co-author on Lecture on: Yesterday’s Collections in Today’s Courses.

6th International Conference on the History of Chemistry, Katholieke Universiteit te Leuven, Belgium, Aug. 28 – Sep. 1, 2007.
Co-author on Lecture on: Trondheim or Oslo? Territories in Early 20th Century Chemistry Education in Norway.

Research Stay, Katholieke Universiteit te Leuven, Belgium, Sep. 3 - 7, 2007.

Conference “Det 18. landsmøte i kjemi”, Lillestrøm, Norway, Oct. 16 – 18, 2007.
Co-author on Lecture on: Trondheim eller Oslo? Kontroversen om retten til å utdanne kjemikere på 1920-tallet.

Meetings at The Niels Bohr Archives and Vitenskapshistorisk Selskab, Copenhagen, Denmark, Nov. 9 – 13, 2007.
Lecture on: Ida Tacke Noddack: Tysk kjemiker på humpete karrierevei.

Meeting at Skolelaboratoriet, NTNU, Dec. 3, 2007.
Lecture on: Skriving som grunnleggende ferdighet og utfordring: Barns og unges vei til ulike fag gjennom skolens skrivekulturer. Skriving i naturfag.

Seminar ”Skrive for å lære – skriving som kunnskapsbygging”, HiST, Trondheim, Norway, Dec. 18, 2007.
Lecture on: Naturfag på mellomtrinn og ungdomstrinn/videregående skole.

**K. Mathisen**

User Meeting Synchrotron Soleil, Paris, France, Jan. 17 – 19, 2007.

Research Stay at the European Synchroton Radiation Facility (ESRF), Swiss-Norwegian Beam Line, Grenoble, France, March 1 – 5, April 12 – 18, June 10 – 22, Sep. 8 – 18, Nov. 19 – Dec. 3, 2007.

Norwegian Synchroton User Meeting, Bergen, Norway, June 4 – 5, 2007.
Lecture on: XAS Studies on Cu:SAPO-5 and Cu:SAPO-11: The Contributory Role of Monomeric Linear Copper(I) Species in the Selective Catalytic Reduction of NOx by Propene.

Norsk katalysesymposium, University of Oslo, Norway, Oct. 23 – 24, 2007.


*Realfagbygget, NTNU*

**Ø. Mikkelsen**

Section Leader, Analytical and Environmental Chemistry Group, Department of Chemistry, NTNU.

Seminar at the Research Council of Norway, Oslo, Jan. 18 – 19, 2007.

Meeting at Lake Biwa Environmental Research Institute, Japan, March 15, 2007.
Co-author on Lecture on: Automatic and unattended Monitoring of Pollutants in Aquatic Systems. This focused on heavy Metals in Lakes and Rivers.

Meeting at Chemical Society of Japan, Osaka, Japan, March 23, 2007.
Co-author on Lecture on: New Methods for automatic and unattended monitoring of heavy Metals.

Meetings to organize Research Co-operation, University of Science and Technology Lille, France, March, 26 – 30, 2007.

Visit at Ecole des Mines de Paris (ARMINS), Paris, France, March 28, 2007.
Lecture on: Monitoring of Environmental Toxicans – Quality Assurance.

Seminar "Gruveforurensning", Løkken, Norway, June 19, 2007.
Co-author on Poster Presentation: Continuous Monitoring of Zinc, Iron and Copper in Raubekken, Løkken verk.

Visit and Presentation of the Lecture "Sensor Development and Automatic Monitoring" for Research Communities in Borne, Netherlands, Sep. 26 – 28, 2007.

Opponent Doctoral Thesis, University of Science and Technology Lille, France, Nov. 13 – 16, 2007.

"POLEKO 2007" International Ecological Fair, Poznan, Poland, Nov. 20 – 23, 2007.
Co-author on Lecture on: Remote Monitoring of Water Quality – Early Warning Systems – Analyzer for Automatic Measurement of Heavy Metals.

**A.R. Moen**

Conference "22. Organisk kjemisk vintermøte", Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentations: "Chemo-enzymatic Methods for Synthesis of Enantiopure Biologically Active Compounds", "Chemo-enzymatic Synthesis of Enantiopure □-Alkyl-□, □-Dihydroxy Units" and "Chemo-enzymatic Synthesis of Enantiopure Alpha-Alkyl-Alpha,Beta-Dihydroxy Units".

**D.G. Nicholson**

Head of the Department of Chemistry

Research stay at the European Synchroton Radiation Facility (ESRF), Swiss-Norwegian Beam Line (SNBL), Grenoble, France, March 1 – 5, April 10 – 15, Sep. 8 – 16, 2007.

Council Meeting SNX (SNBL), Bergen, Norway, June 6 – 10, 2007.

User Meeting, Maxlab, Lund, Sweden, Oct. 28 – 31, 2007.

Research Stay and SNX Council Meeting at the ESRF, SNBL, Grenoble, France, Nov. 23 – 30, 2007.

**C. Nordhei**

Research Stay at the European Synchroton Radiation Facility (ESRF), Swiss-Norwegian Beam Line, Grenoble, France, June 10 – 20 and Sep. 13 – 18, 2007.

Norwegian Synchroton User Meeting, Bergen, Norway, June 4 – 5, 2007.
Lecture on: AXANES and EXAFS Study on Nanophase Nickel, Cobalt and Zinc Ferrite.

**V. Partali**

Conference "22. Organisk kjemisk vintermøte", Røros, Norway, Jan. 11 – 12, 2007.
Co-author on Poster Presentation: Synthesis and Physicochemical Properties of Cationic Surfactants.

Research Co-operation at Heinrich-Heine Univärsitet, Düsseldorf, Germany, May 31 – June 5, 2007.

Research Co-operation at Université de Fribourg, Pérolls, Switzerland, Sep. 7 – 16, 2007.

*Strategy seminar at Jægtvolden, Inderøy*

**A.L. Ramstad**

Section Leader, Physical Chemistry Group, Department of Chemistry, NTNU.

2nd NTNU NanoLab User Meeting 2007, Lerchendal gård, Trondheim, March 7, 2007.
Lecture on: NanoLab's Clean Room for Synthesis by Chemical Methods.
Co-author on Poster Presentation: Surface Self Diffusion of Hydrogen on Carbon Support.

Norwegian Synchroton User Meeting, Bergen, Norway, June 4 – 5, 2007.

Co-organizer of the Conference NANOMAT 2007, Bergen, Norway, June 6 – 7, 2007.
Co-author on Poster Presentation: Surface Self Diffusion of Hydrogen on Carbon Support.

Conference "Diffusion Fundamentals II", L`Aquila, Italy, Aug. 25 – 30, 2007.
Co-author on Poster Presentations: "Surface Self Diffusion of Hydrogen on Carbon Support by Quasielastic Neutron Scattering" and "Dynamical Behaviour of H2 Molecules on Graphite Surface. A Molecular Dynamics Study".

**C. Sanz-Navarro**

3rd NTNU Seminar: Synthesis and Applications of Carbon Nanofibers/Nanotubes, NTNU, Feb. 14, 2007.
Co-author on Lecture on: Molecular Dynamics Simulation of the Binding of Platinum Clusters to Graphite Sheets.

Yale University, New Haven, USA, March 15, 2007.
Co-author on Lecture on: Molecular Dynamics Simulations of Catalytic Activity: Carbon Materials as a Carrier of Platinum Clusters.

Long Time Scale Dynamics Workshop, Loughborough, UK, April 16 – 17, 2007.
Co-author on Poster Presentations: “LargeTime-Scale Protein Dynamics by Strategic
Alteration of the Confirmation of Selected Residues” and “Simulations of Transition-Metal Clusters Adsorbed on Carbon Nanofibers by Using ReaxFF”.

Conference NANOMAT 2007, Bergen, Norway, June 6 – 7, 2007.

4th National FUNMAT Meeting, Bergen, Norway, June 8, 2007.
Co-author on Lecture on: Molecular Dynamics Simulations of Binding of Metal Catalyst Nanoparticles to Carbon Nanostructures by Using ReaxFF.

International Conference on Materials for Advanced Technologies 2007 (ICMAT 2007), Singapore, July 1 – 6, 2007.
Co-author on Lecture on: Molecular Dynamics Simulations of Metal Catalyst Nanoparticles Supported on Carbon Nanostructures by ReaxFF.
Co-author on Poster Presentation: Large Time-Scale Protein Dynamics by Strategic Alteration of the Confirmation of Selected Residues.

13th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis (ISHHC XIII), Berkeley, California, USA, July 16 - 20, 2007.
Co-author on Lecture on: Molecular Dynamics Simulations of Binding of Metal Catalyst Nanoparticles to Carbon Nanostructures by Using ReaxFF.

Conference ”EuropaCat VIII”, Åbo/Turku, Finland Aug. 26 – 31, 2007.
Co-author on Poster Presentation: Carbon Nanofibers as a Platform in Nanocatalysis Engineering.

*Strategy seminar at Jægtvolden, Inderøy*

**R. Schmid**

12th Norwegian Seminar on Mass Spectrometry, Hafjell, Norway, Jan. 22 – 24, 2007.

**K. Schrøder**

Research Co-operation at Warsaw University of Technology, Poland, Feb. 1 – 5, 2007.
Lecture on: New Methods for Automatical and Remotely Controlled Monitoring of Heavy Metals in Waters.

Meeting at Lake Biwa Environmental Research Institute, Japan, March 15, 2007.
Lecture on: Automatic and Unattended Monitoring of Pollutants in Aquatic Systems. This Focused on Heavy Metals in Lakes and Rivers.

Meeting at Chemical Society of Japan, Osaka, Japan, March 23, 2007.
Lecture on: New Methods for Automatic and Unattended Monitoring of Heavy Metals.

Seminar “Gruveforurensning”, Løkken, Norway, June 19, 2007.
Co-author on Poster Presentation: Continuous Monitoring of Zinc, Iron and Copper in Raubekken, Løkken verk.

“POLEKO 2007” International Ecological Fair, Poznan, Poland, Nov. 20 – 23, 2007.
Co-author on Lecture on: Remote Monitoring of Water Quality – Early Warning Systems – Analyzer for Automatic Measurement of Heavy Metals.

**S. Skogvold**

Seminar ”Gruveforurensning”, Løkken, Norway, June 19, 2007.
Co-author on Poster Presentation: Continuous Monitoring of Zinc, Iron and Copper in Raubekken, Løkken verk.

**H.S. Smalø**

Workshop “Norwegian Theoretical Chemistry: From Molecules to Nanostructures”, NTNU, Trondheim, Nov. 8 – 11, 2007.
Co-author on Lecture on: “Electronegativity Equalization Models for Non-Metallic System”.

**A.O. Steen**

European Research Course on Atmospheres, Grenoble, France, Jan. 8 – Feb. 11, 2007.
Co-author on Lecture on: Mercury in the Arctic.

Field Work, Ny-Ålesund, Spitzbergen, April 10 – May 14, June 18 – 28 and Aug. 1 – 6, 2007.

Researcher’s Night, NTNU, Trondheim, Sep. 28, 2007.
Co-author on Lecture on: Kvikksølv i Arktis.

Article in Miljøjournalen: Kvikksølvmysterium i Arktis. Oct. 29, 2007
Workshop "AMAP 2011 Mercury Assessment", Copenhagen, Denmark, Oct. 29 – 31, 2007.
Co-author on Lecture on: AMDE Activities at Ny-Ålesund, Andøya and Troll.

**E. Steinnes**

Det 16. nasjonale seminar om hydrogeologi og miljøkjemi, NGU, Trondheim, Feb. 7 – 8, 2007.
Lecture on: Atmospheric Metal Deposition in Norway 1977 – 2005 Studied by Moss Analysis Using ICP-MS.

20th Task Force Meeting on the UNECE ICP Vegetation, Dubna, Russia, March 5 – 9, 2007.
Co-author on Lecture on: 30 years of Atmospheric Deposition Studies in Norway Using Moss Analysis.
Co-author on Poster Presentation: Epithermal Neutron Activation Analysis of Moss Biomonitors Used to Estimate Metal Pollution in the Surroundings of Thermal Power Plants in Central Russia.

Conference "Norsk-Svensk Miljøkjemisk vintermøte", Geilo, Norway, March 12 – 14, 2007.
Lecture on: 30 Years of Atmospheric Deposition Studies in Norway Using Moss Analysis.

NKS Seminar on Radionuclide Speciation and Radioactive Particle Studies in a Nordic Context, Ås, Norway, April 19 – 20, 2007.
Lecture on: Trace Element Speciation in Aquatic Systems: General Principles and Selected Examples.

Conference "Mountain Areas – Ecological Problems of Cities", Yerevan, Armenia, May 29 – 30, 2007.
Lecture on: Soils and Geomedicine.

32nd International Symposium on Remote Sensing of Environment, San José, Costa Rica, June 25 – 29, 2007.
Lecture on: Soil and Health.

Workshop "Nuclear Physics Methods and Accelerators in Biology and Medicine – 2007", Prague, Czech Rep., July 8 – 19, 2007.
Lecture on: Radioecology.

9th International Conference on the Biogeochemistry of Trace Elements, Beijing, China, July 15 – 19, 2007.
Co-author on Lectures on: "Distribution of 28 Elements in Podzol Profiles Studied by Fractional Extractions and Multivariate Statistics" and "Large-Scale Studies of 137Cs Deposition in Norway from the Chernobyl Accident".

3rd International Conference on Environmental, Health and Safety Aspects Related to Production of Aluminium, Loen, Norway, Sep. 10 – 13, 2007.
Lecture on: Deposition of some Inorganic Pollutants in the Vicinity of Norwegian Aluminium Plants.

12th International Conference on Modern Trends in Activation Analysis, Tokyo, Japan, Sep. 16 – 21, 2007.
Lecture on: INAA of Geological Material Using a Combination of Epithermal Activation and Compton Suppression.

NATO Project, Tbilisi, Georgia, Oct. 7 – 12, 2007.

ISTERH Conference on Trace Elements in Diet, Nutrition & Health, Crete, Greece, Oct. 21 – 26, 2007.
Co-author on Poster Presentations: "A Nation-Wide Survey of Trace Elements in Lynx, Wolverines, Wolves and Brown Bears in Norway", "Trace Elements in Cerebrospinal Fluid and Blood from Patients with a Rare Progressive Central and Peripheral Demyelinating Disease" and "Trace Elements in Serum from Patients with Parkinson's Disease – a Prospective Case-Control Study".

Research Co-operation, Dubna, Russia, Oct. 22 – 29, 2007.

Workshop "AMAP 2011 Mercury Assessment", Copenhagen, Denmark, Oct. 29 – 31, 2007.
Co-author on Lecture on: AMDE Activities at Ny-Ålesund, Andøya and Troll.

LRTAP Convention Workshop on Critical Loads of Heavy Metals, Windermere, UK, Nov. 21 – 23, 2007.
Introductory Talk: Distribution and Fate of Metals Supplied to Norway by Long-Range Atmospheric Transport.
Co-author on Poster Presentation: Heavy Metals in Mosses: Temporal Trends (1990-2000) Across Europe.

*View from Trondheim harbour*

**V. Stockmann**

Conference "22. Organisk kjemisk vintermøte", Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentation: Synthesis of new β–Carboline Analogues.

21st International Congress for Heterocyclic Chemistry, University of New South Wales, Sydney, Australia, July 15 – 20, 2007.
Co-author on Poster Presentation on: Synthesis of new β–Carboline Analogues.

*Kristina working on her data*

**K. Strasunskiene**

Seminar ”Gruveforurensning”, Løkken, Norway, June 19, 2007.
Co-author on Poster Presentation: Continuous Monitoring of Zinc, Iron and Copper in Raubekken, Løkken verk.

Research stay at University of Science and Technology of Lille, France, June 24 – July 20, 2007.

**F. Tjosås**

Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentation: Oxidative Cyclisation of N-Arylaminopyridines.

8th Annual Florida Heterocyclic IUPAC-Sponsored Conference, Gainesville, Florida, USA, March 11 - 14, 2007.
Co-author on Poster Presentation: Synthetic Applications of □-Pyridylmalonates.

**J. Xu**

Joint European Thermodynamics Conference IX, St. Etienne, France, June 12 – 15, 2007.
Co-author on Lecture on: Transport Properties of a Reacting Mixture in a Temperature Gradient as Studied by Molecular Dynamics Simulations.

Conference “Thermodynamics 2007”, Paris, France, Sep. 26 – 28, 2007.
Co-author on Poster Presentation: Transport Properties of a Reacting Binary Fluid, A Non-Equilibrium Molecular Dynamics Simulations Study.

**C.L. Øpstad**

Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 12, 2007.
Co-author on Poster Presentation: Synthesis and Characterisation of Cationic Carotenoid Surfactants.

Research Stay at Weill Cornell Medical College in Quatar, Doha, Quatar, June 4 – 18, 2007.

**J.E. Aaseng**

Conference “22. Organisk kjemisk vintermøte”, Røros, Norway, Jan. 11 – 14, 2007.
Co-author on Poster Presentation: Aziridines from L-Aspartic Acid – Synthesis and Ring Opening Reactions.

**P. – O. Åstrand**

Research Co-operation at University of Copenhagen, Denmark, Jan. 2 – 5, 2007.

3rd NTNU Seminar: Synthesis and Applications of Carbon Nanofibers/Nanotubes, Department of Chemical Engineering, NTNU, Trondheim, Feb. 14, 2007.
Lecture on: Electronic Polarization of Nanotube Aggregates as Calculated by a Point-Dipole Interaction Model.
Co-author on Lecture on: Molecular Dynamics Simulation of the Binding of Platinum Clusters to Graphite Sheets.

Research Co-operation at California Institute of Technology, Pasadena, California, USA, March 2 – 6, 2007.
Lecture on: “Molecular Mechanics Models for Linear and Nonlinear Electronic Polarization”,

Research Co-operation at Northwestern University, Illinois, USA, March 7 – 11, 2007.

Research Co-operation at University of Connecticut, Storrs, USA, March 12 – 13 and June 28 – July 13, 2007.
Lectures on: “Molecular Modelling: Condensed Phases in Strong Fields?” and “Molecular Mechanics Models for Molecular Conductance”

Research Co-operation at Yale University, New Haven, Connecticut, USA, March 14 – 18, 2007.
Lecture on: Molecular Dynamics Simulations of Catalytic Activity: Carbon Materials as a Carrier of Platinum Clusters.

Long Time Scale Dynamics Workshop, Loughborough, UK, April 16 – 17, 2007.
Co-author on Poster Presentation: Simulations of Transition-Metal Clusters Adsorbed on Carbon Nanofibers by Using ReaxFF.

Research Co-operation at Université Joseph Fourier, Grenoble, June 3 – 11, 2007.

4th National FUNMAT Meeting, Bergen, Norway, June 8, 2007.
Co-author on Lecture on: Molecular Dynamics Simulations of Binding of Metal Catalyst Nanoparticles to Carbon Nanostructures by Using ReaxFF.

Research Co-operation at University of Tromsø, Norway, June 13 – 14, 2007.

International Conference on Materials for Advanced Technologies 2007 (ICMAT 2007), Singapore, July 1 – 6, 2007.
Co-author on Lecture on: Molecular Dynamics Simulations of Metal Catalyst Nanoparticles Supported on Carbon Nanostructures by ReaxFF.

13th International Symposium on Relations Between Homogeneous and Heterogeneous Catalysis (ISHHC XIII), Berkeley, California, USA, July 16 - 20, 2007.
Co-author on Lecture on: Molecular Dynamics Simulations of Binding of Metal Catalyst Nanoparticles to Carbon Nanostructures by Using ReaxFF.
Conference ”EuropaCat VIII”, Åbo/Turku, Finland, Aug. 26 – 31, 2007.
Co-author on Poster Presentation: Carbon Nanofibers as a Platform in Nanocatalysis Engineering.

Workshop “Norwegian Theoretical Chemistry: From Molecules to Nanostructures”, NTNU, Trondheim, Nov. 8 – 11, 2007.
Co-author on Lectures on: “Calculation of the Frequency-Dependent Polarizability of Hydrocarbons and Fullerenes Using a Charge-Dipole Model”, “A Study of the Structure of Carbon-Supported Metal Clusters by Molecular Dynamics Simulations” and “Electronegativity Equalization Models for Non-Metallic System”.

Meetings at AIST, Osaka, Japan, Nov. 30 – Dec. 12, 2007.

## Spring examination

| Course no. | Course title (credits) | Lectures and exercise coordinators | Candidates /Passed |
|---|---|---|---|
| RFEL1001 | Natural Science and World Views (7,5) | Reidar Edvald Stølevik<br>Karl Erik Zachariassen | 55/47 |
| KJ1020 | Organic Chemistry (15) | Vassilia Partali | 138/98 |
| KJ2022 | Spectroscopic Methods in Organic Chemistry (7,5) | Elisabeth E Jacobsen | 18/14 |
| KJ2024 | Organic Synthesis, Laboratory (7,5) | Odd Reidar Gautun<br>Anne Fiksdahl | 6/6 |
| KJ2041 | Physical Chemistry II (7,5) | Reidar Edvald Stølevik | 14/13 |
| KJ2043 | Physical Methods in Structural Chemistry (15) | Karina Mathisen<br>Reidar Edvald Stølevik | 9/9 |
| KJ2050 | Analytical Chemistry, Basic Course (7,5) | Øyvind Mikkelsen<br>Florinel Gabriel Banica | 13/13 |
| KJ2053 | Chromatography (7,5) | Anne Fiksdahl<br>Rudolf Schmid | 23/22 |
| KJ2070 | Environmental Chemistry (15) | Torunn Berg<br>Trond Peder Flaten | 39/34 |
| KJ3055 | Analytical Atomic Spectrometry (7,5) | Florinel Gabriel Banica | 4/4 |
| KJ3065 | Enzyme chemistry (7,5) | Torbjørn Ljones | - |
| KJ8100 | Organic Medicinal and Pharamaceutical Chemistry (7,5) | Derek James Chadwick | 27/23 |
| KJ8106 | Advanced Organic Chemistry (7,5) | Per Henning Carlsen | - |
| KJ8200 | Spectroscopy and Chemometrics (7,5) | Bjørn Kåre Alsberg | - |
| KJ8202 | Thermodynamics of Hydrocarbon Mixtures (7,5) | Tore Haug-Warberg | 5/5 |
| KJ8203 | Statistical Thermodynamics and Computer Simulations (7,5) | Per-Olof Åstrand | 4/4 |
| KJ8204 | Quantitative Structure-Activity Relationships (7,5) | Bjørn Kåre Alsberg | - |
| KJ8205 | Molecular Modelling (7,5) | Per-Olof Åstrand | - |
| KJ8208 | Advanced Irreversible Thermodynamics (6) | Signe Kjelstrup | 4/4 |
| TKJ4111 | Organic Chemistry, Advanced Course (7,5) | Bård Helge Hoff | 13/10 |
| TKJ4130 | Organic Synthesis, Laboratory (7,5) | Odd Reidar Gautun<br>Anne Fiksdahl | 4/4 |
| TKJ4135 | Organic Synthesis, Advanced Course (7,5) | Odd Reidar Gautun | 10/7 |
| TKJ4145 | Industrial Organic Chemistry, Research Projects (7,5) | Bård Helge Hoff | 2/2 |
| TKJ4160 | Basic Physical Chemistry and Laboratory (15) | Signe Kjelstrup<br>Per-Olof Åstrand<br>Henrik Koch | 63/45 |
| TKJ4166 | Chemical Bond Theory and Spectroscopy (7,5) | Henrik Koch | 28/22 |
| TKJ4175 | Chemometrics, Basic Course (7,5) | Bjørn Kåre Alsberg | 7/5 |
| TKJ4190 | Physical Chemistry, Project Work (7,5) | Terje Bruvoll | 1/1 |
| TKJ4850 | Experts in Team, Interdisciplinary Project (7,5) | Per-Olof Åstrand | 14/14 |
| TKJ4700 | Physical Chemistry, Specialization (22,5) | | 1/1 |

## Autumn examination

| Course no. | Course title (credits) | Lectures and exercise coordinators | Candidates /Passed |
|---|---|---|---|
| KJ1000 | General Chemistry (15) | Thorleif Anthonsen<br>Torbjørn Ljones<br>Annette Lykknes | 185/168 |
| KJ1030 | Inorganic Chemistry (15) | Astrid Lund Ramstad | 53/47 |
| KJ1040 | Physical Chemistry (15) | Reidar Edvald Stølevik<br>Astrid Lund Ramstad<br>Florinel Gabriel Banica | 51/49 |
| KJ2031 | Inorganic Chemistry, Advanced Course (7,5) | Karina Mathisen | 7/7 |
| KJ2050 | Analytical Chemistry, Basic Course (7,5) | Øyvind Mikkelsen<br>Florinel Gabriel Banica | 9/9 |
| KJ2051 | Analytical Chemistry, Advanced Course I (7,5) | Øyvind Mikkelsen<br>Florinel Gabriel Banica | 6/6 |
| KJ2090 | Chemistry Education - Chemisty Dissemenation (7,5) | Per Odd Eggen | 3/2 |
| KJ2091 | Teacher training/dissemination project in chemistry (7,5) | Lise Kvittingen<br>Per Odd Eggen | 2/2 |
| KJ3021 | Nuclear Magnetic Resonance Spectroscopy (7,5) | Nebojsa Simic | 16/14 |
| KJ3058 | Analytical Chemical Separation Techniques (7,5) | Rudolf Schmid | 1/1 |
| KJ3071 | Applied geochemistry (7,5) | Rolf Tore Ottesen | 6/6 |
| RFEL3093 | Episodes from the history of science | Annette Lykknes<br>Roland Wittje | 3/3 |
| KJ8021 | Stereochemistry and Synthesis of Chiral Compounds (7,5) | Thorleif Anthonsen | 6/6 |
| KJ8026 | Biocatalysis in Organic Chemistry (7,5) | Thorleif Anthonsen | 11/11 |
| KJ8052 | Analytical Electrochemistry and its Application within<br>Industrial and Environmental Monitoring (7,5) | Øyvind Mikkelsen | 3/3 |
| KJ8056 | Chemical and Sensors and Biosensors (7,5) | Florinel Gabriel Banica | 6/6 |
| KJ8070 | Advanced Aquatic Chemistry (15) | Trond Peder Flaten | 10/10 |
| KJ8104 | New Methods in Organic Synthesis (7,5) | Anne Fiksdahl | - |
| KJ8105 | Organometallic Compounds in Organic Synthesis (7,5) | Odd Reidar Gautun | 4/4 |
| KJ8106 | Advanced Organic Chemistry | Per Henning Carlsen | - |
| KJ8206 | Advanced Quantum Chemical Methods (7,5) | Mats Linus Henrik Boman | - |
| KJ8207 | Advanced Microarray Data Analysis (7,5) | Bjørn Kåre Alsberg | 9/8 |
| TKJ4100 | Basic Organic Chemistry and Laboratory (15) | Per Henning Carlsen | 75/45 |
| TKJ4170 | Quantum Chemistry, Advanced Course (7,5) | Mats Linus Henrik Boman | 1/1 |
| TKJ4180 | Physical Organic Chemistry (7,5) | Rudolf Schmid | 13/11 |
| TKJ4185 | Chemical Instrumentation and Experimental Measurements (7,5) | Terje Bruvoll | 2/2 |
| TKJ4195 | Chemometrics, Advanced Course (7,5) | Bjørn Kåre Alsberg | 4/3 |
| TKJ4200 | Irreversible Thermodynamics (7,5) | Torleif Holt | 4/4 |
| TKJ4205 | Computational Chemistry (7,5) | Per-Olof Åstrand | 6/6 |
| TKJ4510 | Physical Chemistry, Specialization Project (15) | Terje Bruvoll | 1/1 |
| TKJ4515 | Physical Chemistry, Specialization Course (7,5) | Terje Bruvoll | 1/1 |
| TKJ4520 | Organic Chemistry, Specialization Project (15) | Odd Reidar Gautun | 1/1 |
| TKJ4525 | Organic Chemistry, Specialization Course (7,5) | Thorleif Anthonsen | 3/3 |

## Re-sit examination

| Course no. | Course title (credits) | Candidates /Passed |
|---|---|---|
| RFEL1001 | Natural Science and World Views (7,5) | 35/33 |
| KJ1000 | General Chemistry (15) | 11/5 |
| KJ1020 | Organic Chemistry (15) | 15/8 |
| KJ1030 | Inorganic Chemistry (15) | 3/2 |
| KJ1040 | Physical Chemistry (15) | 1/0 |
| KJ2020 | Organic Chemistry, Advanced Course (7,5) | 1/1 |
| KJ2053 | Chromatography (7,5) | 2/2 |
| KJ2070 | Environmental Chemistry (15) | 4/4 |
| KJ3021 | Nuclear Magnetic Resonance Spectroscopy (7,5) | 1/1 |
| KJ3058 | Analytical Chemical Separation Techniques (7,5) | 1/1 |
| KJ8056 | Chemical and Sensors and Biosensors (7,5) | 1/1 |
| KJ8070 | Advanced Aquatic Chemistry (15) | 1/1 |
| KJ8100 | Organic Medicinal and Pharamaceutical Chemistry (7,5) | 2/1 |
| KJ8202 | Thermodynamics of Hydrocarbon Mixtures (7,5) | 2/2 |
| KJ8207 | Advanced Microarray Data Analysis (7,5) | 1/1 |
| KJ8208 | Advanced Irreversible Thermodynamics (6) | 2/2 |
| TKJ4100 | Basic Organic Chemistry and Laboratory (15) | 9/5 |
| TKJ4111 | Organic Chemistry, Advanced Course (7,5) | 1/1 |
| TKJ4125 | Natural Products Chemistry (7,5) | 1/1 |
| TKJ4135 | Organic Synthesis, Advanced Course (7,5) | 1/1 |
| TKJ4160 | Basic Physical Chemistry and Laboratory (15) | 9/2 |
| TKJ4166 | Chemical Bond Theory and Spectroscopy (7,5) | 1/1 |
| TKJ4175 | Chemometrics, Basic Course (7,5) | 2/2 |
| TKJ4180 | Physical Organic Chemistry (7,5) | 1/0 |

Willow herb (Epilobium angustifolium)

## Siv.ing. students

**3. year (MTKJ)**
Lyngvi, Eirik
Mekki, Miriam
Seglem, Karen Nessler
Slungård, Sigrid Volden
Takla, Marit
Vågenes, Birgitte Bårli
Willassen, Veronica

**4. year (MTKJ)**
Krakeli, Tor Arne
Kvalvåg, Sondre Schnell
Landsem, Eva
Mui, Vivian Wing Laam
Ringholm, Magnus
Strand, Lilian Helene Sola
Sørensen, Benedicte Riise
Sørum, Christopher
Voldsund, Mari
Wilhelmsen, Øivind
Åstrand, Ove Alexander

**5. year (MTKJ)**
Høgmoen, Hanne
Lervik, Anders
Melnes, Silje


*Teaching laboratory*

## Master students

**Chemistry (MKJ)**
Alsvik, Inger Lise
Berge, May Britt
Berge, Øystein Rønning
Bøyesen, Katrine Lie
Delic, Asmira
Grave, Anlaug Haukvik
Helland, Tone Grangård
Hermann, Solveig
Holt, Yngvil
Hystad, Madeleine
Jonassen, Hilding
Kjøglum, Kristin Tyldum
Lie, Alexander
Lorentzen, Marianne
Lystvet, Sina Maria
Martinsen, Morten
Martinsen, Thomas
Møllegård, Ståle
Neerland, Elisabeth
Næss, Mari Kirkebøen
Siegesmund, Øyvind Torbjørn
Skårn, Jenne Skeide
Sørensen, Kari Bjerke
Tjemsland, Johanne Marie
Valvik, Beate
Aaen, Ingrid

**Environmental toxicology and chemistry (MFORU)**
Holsen, Aase Marie Hersleth
Ottemo, Vivian Grønhaug

**Natural resource mangagement (MNATR)**
Eliassen, Ragnhild Oline
Salomonsen, Silje Naper

**Master of Science Education (MLREAL)**
Bjørk, Tina Beate
Brimi, Aslak Opsahl
Elgen, Marianne
Frøland, Stine Lindset
Hansen, Mari Roen
Hole, Marianne Prestvik
Valved, Hilde

## PhD in Chemistry

| | |
|---|---|
| **Buttingsrud, Bård** | **An improved method for comparing the 3D electronic structure of molecules in rational drug design.** |
| Trial lecture | Searching for new drugs using combinational chemistry |
| Supervisor | Professor Bjørn Kåre Alsberg |
| Evaluation committee | Reader Dr. Paul Popelier, Manchester Interdisciplinary Biocentre (MIB), University of Manchester<br>Research Associate Dr Amanda Clare, Department of Computer Sience, University of Wales<br>Professor Reidar E. Stølevik, Institutt for kjemi, NTNU |
| **Gidskehaug, Lars** | **Development of chemometric methods for variable selection on microarray data.** |
| Trial lecture | Variable selection in high-throughput data problems |
| Supervisor | Professor Bjørn Kåre Alsberg |
| Evaluation committee | Assistant Professor PhD Johan Westerhuis, Universiteit van Amsterdam Swammerdam, Institute for Life Sciences Biosystems Data Analysis, Amsterdam, The Netherlands<br>Postdoc, PhD Solve Sæbø, Institutt for kjemi, bioteknologi og matvitenskap, Universitet for miljø og biovitenskap, Ås<br>Professor Henrik Koch, Institutt for kjemi, NTNU |
| **Kildahl-Andersen, Geir** | **Polyenyl cations and radical cations - synthesis, spectroscopic properties and reactions.** |
| Trial lecture | Chemical Aspects of Photodynamic Cancer Therapy |
| Supervisor | Professor Thorleif Anthonsen, Institutt for kjemi, NTNU |
| Evaluation committee | Professor Dr. Johan Lugtenburg, Gorlaeus Laboratories, University of Leiden, RA Leiden, The Netherlands<br>Professor Arne Jørgen Aasen, Farmasøytisk institutt, Universitetet i Oslo<br>Førsteamanuensis Dr. Eva H. Mørkved, Institutt for kjemi, NTNU |
| **Meland, Anne-Kristine** | **Impedance Diagrams of the Electrodes in the Polymer Electrolyte Membrane Fuel Cell.** |
| Trial lecture | Electrochemical reduction of carbon dioxide. Fundamentals and applications |
| Supervisor | Professor Signe Kjelstrup |
| Evaluation committee | Professor dr.tekn. Göran Lindbergh, Kjemiteknikk, Kungliga Tekniska högskolan, Stockholm<br>Seniorforsker dr. Børre Tore Børresen, Statoil forskningssenter ASA, Rotvoll<br>Professor dr.ing. Svein Sunde, Institutt for materialteknologi, NTNU, Trondheim |
| **Moen, Anders Riise** | **Enzymatic asymmetrization and kinetic resolution. Synthesis of drug precursors, natural products and carbohydrates.** |
| Trial lecture | Asymmetrisk organokatalyse og aldolreaksjonen; betydning for homokiralitet i naturen? |
| Supervisor | Professor Thorleif Anthonsen |
| Evaluation committee | Dr. Poul B. Rosenius Poulsen, New Business Discovery Novozymes, Denmark<br>Professor Arne Jørgen Aasen, Farmasøytisk institutt, Univeristetet i Oslo<br>Professor Torbjørn Ljones, Institutt for kjemi, NTNU |
| **Rye, Morten Beck** | **Image segmentation and multivariate analysis in two-dimensional gel electrophoresis.** |
| Trial lecture | An overview of the Ogston model and its applications in protein gel electrophoresis |
| Supervisor | Professor Bjørn Alsberg |
| Evaluation committee | Associate Professor PhD Ib Søndergaard, Danmarks Tekniske Universitet, BioCentrum-DTU, Kgs. Lyngby, Danmark<br>Professor PhD Tormod Næs, Matforsk AS, Ås<br>Professor PhD Per-Olof Åstrand, Institutt for kjemi, NTNU |

| | |
|---|---|
| **Tjosås, Freddy** | **Nitropyridines and pyridyl malonate derivatives in heterocyclic chemistry.** |
| Trial lecture | Gullkatalyserte reaksjoner i organisk syntese |
| Supervisor | Professor Anne Fiksdahl |
| Evaluation committee | Professor Kristina Luthman, Institutionen för kemi, Läkemedelskemi, Göteborgs universitet, Sverige<br>Førsteamanuensis Tore Hansen, Kjemisk institutt, Universitetet i Oslo<br>Førsteamanuensis Odd Reidar Gautun, Institutt for kjemi, NTNU |

## Cand.scient in Chemistry 2007

| | |
|---|---|
| **Azizyan, Mahnaz** | **Studier av human mitokondriell uracil-DNA glukosylase UNG1**. |
| Supervisors: | Professor Geir Slupphaug<br>Professor Thorleif Anthonsen |
| Examiner: | Dr. Ingrid Eftedal. |

| | |
|---|---|
| **Bergene, Nina Iren** | **Rensing og karakterisering av AlgL fra Pseudomonas fluorescens, og forsøk på etablering av et in vitro-system for alginatsyntese** |
| Supervisors: | Research officer Helga Ertesvåg<br>Professor Svein Valla<br>Professor Thorleif Anthonsen |
| Examiner: | Associate Professor Kåre Haugan |

| | |
|---|---|
| **Storstad, Trond Magne** | **Tungmetaller i viltvoksende norske matsopper** |
| Supervisors: | Professor Steinnes, Eiliv<br>Adviser Bjørn Ove Berthelsen |
| Examiner: | Supervisor Per Varskog |

*Daffodils outside the departement*

## MSc in Chemistry/Siv.ing. 2007

| | |
|---|---|
| **Siv.ing. Ane Arstad** | **Synthesis of new tripodal chelators for complexation of actinides and latinides** |
| Supervisor: | Associate Professor Bård Hoff and Research Scientist Bror Johan Wik |
| Examiner: | Associate Professor Trond Vidar Hansen |
| **Siv.ing. Kristine Løland Eriksen** | **Synthesis of beta-carbolin analogues** |
| Supervisor: | Professor Anne Fiksdahl |
| Examiner: | Professor Jan Skramstad |
| **Siv.ing. Ingvild Eide-Haugmo** | **Preparation and characterization of polymermatrixes for use in composite fuel** |
| Supervisor: | Associate Professor Rudolf Schmid and Research Scientist Erik Unneberg |
| Examiner: | Associate Professor Per Ola Rønning |
| **Siv.ing. Ivar Brøndbo Kjerstad** | **Cyclisation reactions for the making of 6-azaindoles and oxazolopyridines** |
| Supervisor: | Professor Anne Fiksdahl |
| Examiner: | Associate Professor Kåre B Jørgensen |
| **Siv.ing. Maria Førde Møll** | **Synthesis and analysis of alfa-fluorophenylethanones and alfa-fluorophenylethanols** |
| Supervisor: | Associate Professor Bård Helge Hoff |
| Examiner: | Dr.scient. Viggo Waagen |
| **Siv.ing. Alexander Nicolaisen** | **Synthesis of polyheterocyclic compounds from pyridylmalonate** |
| Supervisor: | Professor Anne Fiksdahl |
| Examiner: | Professor Jan Skramstad |
| **Siv.ing. Gard Reian** | **Asymmetric catalytic aziridination of alkenes for the purpose of manufacturing substituted 2-aminotetralines** |
| Supervisor: | Associate Professor Odd Reidar Gautun |
| Examiner: | Associate Professor Trond Vidar Hansen |
| **Siv.ing. Solrun Johanne Vevelstad** | **Syntetic studies towards piperazinomycin** |
| Supervisor: | Associate Professor Odd Reidar Gautun |
| Examiner: | Associate Professor Kåre B Jørgensen |
| **Juan Francisco Insua Peres**<br>(Sokrates student) | **Synthesis of polyheterocyclic compounds from pyridylmalonate** |
| Supervisor: | Professor Anne Fiksdahl |
| Examiner: | Professor Emeritus Jan Magnus Bakke |

## MSc in Chemistry 2007

| | |
|---|---|
| **Angelsen, Ragnhild Beate Strand** | **Undersøking av det aktive senteret til lipase A frå Candida antarctica.** |
| Supervisor: | Professor Thorleif Anthonsen |
| Examiner: | Associate Professor Eirik Sundby |
| | |
| **Drange, Kristine** | **Specieringstudier av aktuelle spormetaller, i vann og sedimenter i brakkvannsone - utvikling av analysemetodikk** |
| Supervisors: | Professor Øyvind Mikkelsen<br>Professor Knut Henning Schrøder |
| Examiner: | Senior Research Fellow Kalman Nagy |
| | |
| **Frigstad, Marte Marie Hansen** | **Kjemo-enzymatisk syntese av iminosyklitol, potensiell hemmer av glykosidaser og glykosyltransferaser** |
| Supervisor: | Professor Thorleif Anthonsen |
| Examiner: | Professor Arne Jørgen Aasen |
| | |
| **Halkjelsvik, Anveig Bjordal** | **Industriell påverknad av elvesletter langs Driva** |
| Supervisors: | Professor Eiliv Steinnes<br>Adjunct Professor Rolf Tore Ottesen |
| Examiner: | Supervisor Per Varskog |
| | |
| **Midtaune, Håkon** | **Kjemoenzymatisk syntese av enantiomert rene byggesteiner basert på para-hydroksypropiofenon** |
| Supervisor: | Professor Thorleif Anthonsen |
| Examiner: | Associate Professor Trond Vidar Hansen |
| | |
| **Nordløkken, Marit** | **Artsforskjeller i konsentrasjon av 56 elementer i naturlig vegetasjon i Sør-Rogaland** |
| Supervisor: | Professor Eiliv Steinnes |
| Examiner: | Adviser Bjørn Ove Berthelsen |
| | |
| **Tronstad, Ingvild** | **Bestemmelse av tungmetaller i elvevann ved bruk av ICP-MS og DGT analyser. Sammenligning mot nyutviklet metode for automatisert tungmetall analyse for bruk i felt** |
| Supervisor: | Professor Øyvind Mikkelsen<br>Professor Knut Henning Schrøder |
| Examiner: | Senior Research Fellow Kalman Nagy |

## MSc in Education, Chemistry

| | |
|---|---|
| **MSc Tonje Birgitte Østebrød** | **Utvikling av metode for forutsigelse av jordskjelvaktivitet ved hjelp av automatisk overvåking av tungmetallkonsentrasjonen i grunnvann** |
| Supervisor: | Professor Øyvind Mikkelsen<br>Professor Emeritus Knut Schrøder |
| Examiner: | Senior Research Scientist Kalman Nagy |

## The following PhD-projects are in progress:

| Student | Title | Thesis advisor |
|---|---|---|
| Andreassen, Trygve | Assymetriske ene-reaksjoner med aza-analoger til svoveldioksid. | Odd Reidar Gautun |
| Boman, Mats Henrik Linus | Analytical coupled-cluster calculation of gauge invariant optical properties. | Henrik Koch |
| Burheim, Odne Stokke | Elektronisk utfelling av jern. (Electrowinning of iron from chloride melts) | Signe Kjelstrup |
| Chu, Chunmei | Automated de novo Optimization of Functional Organometallic Compounds by Integrating A OSAR/Genetic Algorithm Method. | Bjørn K. Alsberg |
| Eggen, Per-Odd | Current chemistry – learning and teaching electrochemistry by experiments. | Lise Kvittingen |
| Esmurziev, Aslan | Synthesis of new fluorinated uronic acids and total synthesis of new uridine diphosphate fluoro-uronic acids. (Syntese av fluorerte uronsyrer og talsyntes av nye uridine difosfat fluoro-uronsyrer.) | Bård Helge Hoff |
| Flatberg, Arnar | Simulation of microarray experiments and protsomic 2D gel electrophoresis. | Bjørn K. Alsberg |
| Fuglseth, Erik | New chiral and fluorinated aromatic compounds. (Nye kirale og fluorere aromatiske forbindelser.) | Bård Helge Hoff |
| Gebremariam, Kidane Fanta | Analytical Methods for Art objects Investigation | Lise Kvittingen |
| Gellein, Kristin | Trace elements and health – in vitro, experimental animal and human population studies. | Trond Peder Flaten |
| Glavatsky, Kirill Sergeevich | Multi-component evaporation as described Using the Nonequilibrium van der Waals square gradient model. | Dick Bedeaux |
| Gonzalez, Susana Villa | Synthesis of optically active surfactants and the study of their properties. | Per H. Carlsen |
| Haas, Ole-Erich | Transport on a nanoscale; at surfaces and contact lines in PEM fuel cells. | Astrid Lund Ramstad |
| Hestad, Øystein Leif | Elektroniske prosesser i frosne dialektriske væsker under høg elektrisk feltpåkjenning. | Per-Olof Åstrand |
| Ingebrigtsen, Stian | Elektroniske prosesser i flytende dielektrika under høye elektriske feltpåkjenninger. (Electronic process in liquid dielectrics under high electric field stress.) | Per-Olof Åstrand |
| Inzoli, Isabella Maria | Molecular modelling of coupled transport of heat and mass. | Signe Kjelstrup |

| | | |
|---|---|---|
| Jartun, Morten | Urban risk – Dispersion mechanisms and possible health effects of PCB in the urban environment. | Eiliv Steinnes |
| Kumelj, Tjasa | Free energy calculations of ligand-protein interactions. | Per-Olof Åstrand |
| Løkken, Torbjørn Vegard | Analyser av vannduggpunkt og hydrokarbonduggpunkt i naturgass. (Determination of water dewpoint and hydrocarbon dewpoint in natural gas.) | Rudolf Schmid |
| Nordhei, Camilla | Structural Studies of Functional Oxides and their Catalytic Behaviour – XAS and XRD Studies of Nanophase Spinels. | Astrid Lund Ramstad |
| Ryeng, Einar | Analyse av mikromatrisedata med induktiv logikk-programmering. | Bjørn K. Alsberg |
| Sandru, Eugenia-Mariana | Synthese av høy umettete bioorganiske forbindelser. (Synthesis of highly unsaturated bioorganic compounds.) | Vassilia Partali |
| Skogvold, Silje Marie | Overvoltage in Voltammetry; Fundamental Processes, related to Analytical Sensor Development for Online and Remote Trace Analyses. | Øyvind Mikkelsen |
| Smalø, Hans Sverre | Molecular models of electronic processen in liquids. | Per-Olof Åstrand |
| Steen, Anne Orderdalen | Atmosfærisk spesiering av kvikksølv i polare områder. | Torunn Berg |
| Stockmann, Vegar | Synthetic Applications of Nitropyridine Derivates. | Anne Fiksdahl |
| Strasunskiene, Kristina | Automatically measuring systems for heavy Metals and trace Metals in waste water from sewage discharge and incineration plants. Early warming systems. | Øyvind Mikkelsen |
| Svendsen, Monica Lian | Systemanalyse av metallforurensning i det terrestriske miljø i Odda-området. | Eiliv Steinnes |
| Xu, Jing | A Nonequilibrium Molecular Dynamics Simulation Study of Chemical Reactors. | Signe Kjelstrup |
| Yu, Qiang | Synthesis of Nucleic Base containing oligomers and polymers. | Per H. Carlsen |
| Øpstad, Christer Lorentz | Synthesis and properties of hydrophilic higly unsaturated amphiphiles for gene transfer. | Vassilia Partali |
| Aarhaug, Thor Anders | Ny membran for polymer brenselsceller. | Signe Kjelstrup |
| Aaseng, Jon Erik | Asymmetric synthesis of substituted 2-aminotetralins. (Asymmetrisk syntese av substituerte 2-aminotetraliner.) | Odd Reidar Gautun |

## Student Exchange from NTNU, Department of Chemistry 2007

| Name | Specialization | Level | Institution |
|---|---|---|---|
| Hystad, Madeleine | BKJ-Struct.chem. | BSc, 3th yr | University of British Colombia, Canada |
| Høyvik, Ida-Marie | BKJ-Struct.chem. | BSc, 3th yr | University of California, Berkeley, USA |
| Åstrand, Ole Alexander | MTKJ-Fys.chem. | MSc, 4th yr | University of California, Berkeley, USA |
| Høgmoen, Hanne | MTKJ-Org.chem. | MSc, 5th yr | University of California, Berkeley, USA |

## Student exchange to NTNU, Department of Chemistry 2007

| Name | Institution |
|---|---|
| Ausin, Maider Reguera | University of the Basque Country, Spain |
| Barras, Mathieu | Université de Technologie de Troyes, France |
| Bõhme, Alexandra | Martin-Luther-University Halle-Wittenberg, Germany |
| Ciftja, Arlinda | University of Tirana, Albania |
| Corcostegui, Cecilia | University of the Basque Country, Spain |
| Einarsdóttir, Dóróthea | University of Iceland, Iceland |
| Exner, Alexander | Universität Hamburg, Germany |
| Hauge, Drew Allen | University of Minnesota, USA |
| Holler, Jes Gitz | Danish University of Pharmaceutical Science, Denmark |
| Lesven, Ludovic | University of Lille, France |
| Louriño Cabana, Beatriz | Universidad de la Coruña, Spain |
| De Meester, Raf Homer Ghislena | Ghent University, Belgium |
| Rennebaum, Sandra | RWTH Achen University of Technology, Germany |
| Rueda Verano, Maria Jesus | University of Cadiz, Spain |
| Schwidom, Dirk | Universität Hamburg, Germany |

*Bumble bee at work*

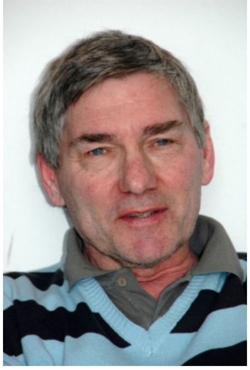
# Academic Staff

## Organic Chemistry


Group Leader
Professor, Dr.ing.
Anne Fiksdahl


Adjunct Professor, Ph.D.
(Oxford) . Derek Chadwick


Professor, Dr.rer.nat.
(Fribourg). Vassilia Partali


Professor, Dr.ing.
Thorleif Anthonsen


Associate Professor, Dr.ing.
Odd Reidar Gautun


Associate Professor, Dr.rer.nat.
(Zürich). Rudolf Schmid


Professor, Ph.D. (Buffalo).
Per Carlsen


Associate  Professor, Dr.scient
Bård Helge Hoff


Associate Professor
Nebojsa Simic

## Physical Chemistry


Group Leader
Associate Professor, Dr.scient.
Astrid Lund Ramstad


Professor, Dr.philos.
Kolbjørn Hagen


Professor, Dr.philos.
Reidar Stølevik


Professor, Dr.scient.
Bjørn Alsberg


Professor, Dr.techn.
Signe Kjelstrup


Professor, Ph.D. (Lund)
Per-Olof Åstrand


Adjunct Professor, Dr.philos.
(Utrecht). Dick Bedeaux


Professor, Ph.D. (Århus).
Henrik Koch


Associate Professor
Morten Bjørgen


Assistant Professor
Terje Bruvoll


Professor, Ph.D.
Torbjørn Ljones

## Environmental and Analytical Chemistry


Group Leader
Dr.Scient
Øyvind Mikkelsen


Professor, Dr.scient.
Lise Kvittingen


Professor, Dr.philos.
Knut Schrøder


Associate Professor, Dr.ing.
Florinel G. Banica


Ph.D.
Karina Mathisen


Professor, Dr.philos.
Eiliv Steinnes


Professor, Dr.scient.
Torunn Berg


Professor, Ph.D. (London)
David Nicholson


Associate Professor, Dr.scient,
Annette Lykknes


Associate Professor, Dr.ing.
Trond Peder Flaten


Adjunct Professor
Rolf Tore Ottesen

## Administrative staff


Head of administration
Anne Langseth


Senior consultant
Lillian Hanssen


First secretary
Aase Sæther


Consultant
Inger Marie Frøseth


Consultant
Ingrid Kristine Tømmerdal

## Technical staff


Senior Technician
Stein Almo


Chief Technician
Julie Jackson


Technician
Nina Klausen


Chief Technician
Syverin Lierhagen


Chief Technician
Tron Rolfsen


Technician
Kari Tanem


Technician
Kjersti Ljones


Technician
Gunnar Svare


Technician
Roger Aarvik

## Temporary Lecturers

Hårklau, Halvard
Jacobsen, Elisabeth E.

## Scientific Assistants

Alsvik, Inger Lise
Andreassen, Trygve
Angelsen, Ragnhild Strand
Bjørk, Tina Beate
Bolstad, Kjersti H.
Breivik, Åshild S.
Eliassen, Ragnhild
Egede-Nissen, Cecilie
Fuglseth, Erik
Grave, Anlaug H.
Haas, Ole-Erich
Hansen, Mari Roen
Holt, Yngvil
Lystvet, Sina
Neerland, Elisabeth
Siegesmund, Øyvind
Steen, Anne O.
Storstad, Trond Magne
Valved, Hilde
Øpstad, Christer L.
Øvergård, Tommy
Aaseng, Jan Erik

## Demonstrators (Master Students)

Angelsen, Ragnhild Strand
Bjørk, Tina Beate
Braaten, Hans Fredrik
Elgen, Marianne
Eliassen, Ragnhild
Esmurziev, Aslan
Finnstun, Elin
Frafjord, Anders Malm
Frigstad, Marte M. Hansen
Frøland, Stine Lindset
Gebremariam, Kidane Fanta
Helgerud, Trygve
Hermann, Solveig
Johansen, Hege D.
Jonassen, Hilding
Karstensen, Kristin
Kvitvang, Hans Fr.
Landsem, EvaLervik, Anders
Lie, Aleksander
Lieungh, Ida
Lorentzen, Marianne
Lyngvi, Eirik
Martinsen, Morten
Martinez, Marcus C.
Melnes, Silje
Midtaune, Håkon
Ringholm, Magnus
Sivertsen, Sveinung
Skårn, Jenny Skeide
Slungård, Sigrid V.
Smørvik, Marte S.
Strand, Lilian H.E.
Sørgård, Hanne
Wiik, Siv Åshild
Wilhelmsen, Øivind
Øverby, Anders

## Guest professors/researchers/lecturers

| | |
|---|---|
| James Burger | Jan. 1 – June 30, 2007 |
| Alexander Mayer | Jan. 15 – 19, 2007 |
| Gabriel Billon | Jan. 29 – Feb. 2, 2007 |
| Olga Safanova | June 23 – 28, 2007 |
| Donald L. Macalady | Aug. 13 – Nov. 30, 2007 |

Director of the Novartis Foundation, London, UK and Adjunct
Professor at Department of Chemistry, NTNU, Derek Chadwick March 8, 2007
“Challenges for the Pharmaceutical Industry”

Research Scientist Christian Collin-Hansen, Statoil, Trondheim March 8, 2007
“The big Questions about Global Warming – and how
Chemists might provide the Answer”

Professor Jürgen Heck, Universität Hamburg, Germany March 13, 2007
Socrates Lecture I: Organometallic Catalysis:
“Transformations of Coordinated Cyclooctatetraene”

Professor Jürgen Heck, Universität Hamburg, Germany March 14, 2007
Socrates Lecture II: Organometallic Catalysis:
“Structure Property Relationships in Dipolar
Organometallic Compounds”

Director of Research Anne-Marie Caminade,
CNRS Toulouse, France Sept. 25, 2007
“Phosphorous Dendrimers – Synthesis, Reactivity,
Properties”

Research Scientist Jenny Beckman, University of Uppsala, Sweden
“Biologihistorie 1 – Ordning og utvikling” Oct. 18, 2007
”Biologihistorie 2 – Molekyler og miljø Oct. 19, 2007

Dr. Slawomira Skrzypek, University of Lodz, Poland Oct. 22, 2007
“Compounds included Guanidine Group as Catalysts
for Hydrogen Reduction at a Mercury Electrode:
Application in Analysis of Pharmaceuticals in Biological Samples”

Photo: David Nicholson og Stein Almo
Layout: Stein Almo

# Annual Report for Department of Chemistry 2007

NTNU
Innovation and Creativity

**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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Norway

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**www.ntnu.no/kjemi**