

Chimia 57 (2003) 62–65
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 ISSN 0009–4293

Focal Point: Fall Meeting of the Swiss Chemical Society (SCS)[§]

October 17, 2002

Organized by: Division of Chemical Research of the SCS^a
 Prof. Wolf-D. Woggon^{b*}, Chairman Local Organizing Committee

Keywords: Fall meeting · Paracelsus Prize · Swiss Chemical Society · Werner Prize

Once again the call for papers for this 2002 meeting was a great success, exceeding with more than 300 papers and more than 700 participants even the previous record of the fall meeting 2001 in Zürich (with about 290 papers). The scientific oral sessions attracted many young people and led to lively discussions. The poster sessions were also well attended, in a nicely organized area, with greatly appreciated sandwiches, juices, coffee and tea for lunch provided very generously by the organizers and hosts in Basel.

The contributions were generally of very high quality – and in part truly exceptional. It is only possible to mention a few highlights here, with apologies to the authors of many outstanding papers which cannot be mentioned here.

From the organizational side there had been some difficulties in the transition from the collaboration with the traditional



André Merbach and Jérôme Lacour

ILMAC to the new R+D in life sciences fair. This principally concerned the organizers, but some members of the Swiss Chemical Society, who did not get the promised free entrance as easily as usual, may also have been affected. We apologize in the name of the fair for any inconveniences that may have arisen, but hope that all matters could be settled satisfactorily in the end.

One of the novelties this year was ‘The Swiss Young Chemists’ Committee’s Career Fair’ which was an outstanding success.

As is the tradition, the meeting started with the presentation (by president *André Merbach*) of the **Werner Prize** 2002. This year the prize was awarded to two young chemists, *Jérôme Lacour* from the Département de Chimie Organique de l’Université de Genève and *Werner Nau* from the Insti-



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tut für Physikalische Chemie, Universität Basel. Jérôme Lacour received the prize ‘in recognition of his valuable contributions to asymmetric synthesis with chiral anions’ and Werner Nau ‘for his outstanding work in the development of intelligent probes for supramolecular and biomolecular probes’. Both laureates presented their work in short lectures. As these will appear in full in later issues of *Chimia*, we will resist the temptation to go into any further detail here.

After this initial high point of the meeting, the scientific sessions continued in several parallel sessions, both scientific and ‘administrative’. It seems that science attracted clearly more people than science administration. The general assemblies of the divisions were poorly attended and will receive no further comment here, except that we note this as a positive sign that firstly shows that it is still science itself which

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[§]Summary by Ruth Schüpbach from recollections of Heinz Berke, Claude Daul, Wolfgang Froestl, Paul Pregosin, Philippe Renaud, John Robinson, Jean-Luc Veuthey, Helma Wennemers, Joggi Wirz, Wolf Woggon, Renato Zenobi.

counts, and secondly that there are fortunately no current administrative controversies of any importance in the society.

As far as science goes, once again, **Computational Chemistry** attracted many of the young people with eleven lectures and eleven posters. Many of the results presented were based on density functional theory applied to molecular science as well as to life science. The prize for the best oral paper was awarded to *Ute F. Röhrig* from the Laboratory of Inorganic Chemistry at ETH Zürich (with M. Parrinello, ETH and CSCS and U. Röthlisberger, now EPFL, as 'senior scientists'). She introduced the chemistry of the 'vision process' and showed how she tries to model the photo-reaction of rhodopsin in a biological environment by a QM/MM approach. Another interesting talk by *Clemence Corminboeuf* about aromaticity questioned a statement by P. Fowler, that the ring current is nearly completely determined by the HOMO. She confirmed with several examples her hypothesis that the lowest π -orbital is of more importance. The prize for the best poster went to *Delphine Bas*, Université de Genève. These papers should be presented in more detail in future issues of CHIMIA. Most of the contributions in these sessions originated from research groups in the western parts of Switzerland, although computational chemistry is well rooted in all parts of the country. Efforts should be made to stimulate 'missing groups' to contribute.

Among the highlights in the **Physical Chemistry** section chaired by Jakob Wirz were the new infrared spectroscopic techniques reported by *Michael Hippler*, this year's Ruzicka prize winner, with applications to the ever-important benzene molecule. Chirality was in the focus of three contributions in this session. *Davide Ferri*, *Thomas Bürgi*, and *Alfons Baiker* from ETH Zürich reported new chirally modified catalysts studied by *in situ* IR-spectroscopy, *Sieghard Albert* from ETHZ reported an outstanding high resolution infrared spectroscopic analysis of CDFCIBr, a classical chiral prototype molecule, and *Achim Sieben* from ETH told us about very new and exiting results of isotope effects in parity violation in chiral molecules, a topic which leads into completely new areas of research on molecular chirality.

The second Physical Chemistry Session chaired by Werner Nau was opened by *David Schürch* from the University of Bern, who reported on the development and optimization of the AgCl photoanode suitable for oxidation of water to oxygen. His excellent talk was selected as the best oral presentation of the physical chemistry ses-

sions. *Claudia Leiggener* and *Huub Maas*, both University of Bern, presented two additional projects from the Calzaferri group. The talk by Leiggener dealt with the spectroscopic properties of silver sulfide-zeolite composites, which display color variations in dependence on the stoichiometry of the silver sulfide. The presentation by Maas described recent developments in the use of dye/zeolite composites as antenna systems for energy trapping. The following paper by *Ana Morandeira*, University of Geneva, was devoted to the study of ultrafast charge transfer processes between singlet-excited acceptor molecules and the solvent as electron donor. *Cosmina Dutan*, also University of Geneva, presented a joint experimental and theoretical project: The EPR and ENDOR spectra of an important class of siloxane radical anions were interpreted and compared with the predictions of DFT calculations for various radical anion geometries. The physical chemistry session was closed by a talk of *J.-D. Grunwaldt*, ETH Zürich, on the technique of *in situ* X-ray absorption and its application for the optimization and mechanistic understanding of heterogeneous catalysis.

The Division of **Analytical Chemistry** continues to grow and had a total of 40 posters and six oral presentations in the Symposium held both in the morning and in the afternoon of October 17, 2002. Posters were on display all day but mostly viewed during a stand-up lunch. The oral presentations started after the General Assembly of the Members of the Division of Analytical Chemistry.

The first invited speaker was Prof. *Barry L. Karger* from the Barnett Institute, Northeastern University, Boston/USA. His talk was entitled 'Recent Advances in High Performance LC (1D and 2D)/Mass Spectrometry for Proteomic Analysis'. The talk covered a lot of ground, from laser capture microdissection as a sample preparation method to multidimensional chromatography to interfacing chromatographic separations with matrix-assisted laser desorption/ionization (MALDI) mass spectrometry. As opposed to mainstream LC/MS, mostly done with atmospheric pressure ionization interfaces such as electrospray, Karger's group advocates an off-line deposition of the effluent on a target plate, followed by MALDI mass spectrometry. The advantage of this approach is the ability to come back to an interesting spot on the sample to perform detailed analyses, combined with the fact that one obtains an archive of the chromatogram in the form of MALDI bands on the target.

This was followed with a presentation given by *Sebastian Friess* from the ETH

Zürich on 'Intrinsic Mass Signal Intensities of Protein Digests'. He presented an interesting hypothesis, namely that the relative MALDI signal intensities of peptide mixtures produced from tryptic digestion of proteins – including effects that are often interpreted being due to signal suppression – are merely a function of the peptide's propensity to form ions in MALDI mass spectrometry. The hypothesis clearly needs to be tested further, but challenges the accepted view about the strongly varying signal intensities in tryptic digests.

Laurent Geiser from the University of Geneva spoke on 'Non-aqueous Capillary Electrophoresis – Electrospray-Mass Spectrometry for the Analysis of Pharmaceutical Compounds'. He presented some interesting findings relating to elution order and peak resolution in electrophoretic separations depending on the physico-chemical properties of the buffer. Many of the observed trends were accurately predicted by a theoretical model developed by the Geneva group. Applications of non-aqueous CE to the analysis of drugs (anti-depressants, amphetamines, beta-blocker) and an outlook of interfacing this separation method with mass spectrometry concluded this presentation.

The second invited speaker was Prof. *Gérard Hopfgartner* from the University of Geneva. 'New Opportunities for the Characterization of Small Molecules and Peptides using Multidimensional Chromatography and Hybrid Tandem Mass Spectrometry'. Hopfgartner has recently joined the University of Geneva, coming from a position at Roche (Basel). Part of the work he presented was based on his previous research in industry and some of it was even confidential. Hopfgartner uses some very powerful LC-MS and LC-MS/MS methods for the unambiguous characterization and quantification of small molecules – many of them metabolites – in complex biological matrices. The methodology combines multidimensional HPLC with microbore or nanobore columns and tandem MS instrumentation, in particular the new hybrid RF/DC quadrupole – linear ion trap mass spectrometer.

Marcel Guillong from the ETH Zurich gave an excellent presentation entitled 'LA-ICP-MS: Particle Composition and their Contribution to Sensitivity and Accuracy of the Method'. The complicated abbreviation is short for Laser Ablation – Inductively Coupled Plasma – Mass Spectrometry, in other words, a combination of the trendiest sample delivery method (by laser ablation on virtually any material) with the workhorse method for elemental and trace analysis, ICP-MS. While nebu-

lization of liquid samples is still the most widely practiced and also the best way to achieve high accuracy and low detection limits in ICP-MS, laser ablation has great promise for localized analyses, for studying heterogeneous materials, and generally for *in situ* analyses without tedious sample preparation steps. However, sample delivery by laser ablation still suffers from some discrimination and fractionation effects. Guillon showed convincingly that the production of aerosol particles from the laser-sample interaction is key to understanding and minimizing these effects. He and his colleagues used aerosol sizing methods to study aerosol formation and transport, and clever ways to influence the size distribution for assessing the effect of aerosol size on ion formation efficiency. Marcel Guillon won the award for the best oral presentation for his talk.

The concluding presentation was given by Dr. *Joachim Mohr* from the EMPA Dübendorf, Switzerland, on 'On-Line Gas Analysis for Process Diagnostics in Semiconductor Industries'. Mohr showed a less widely known method, on-line infrared spectroscopy, for the analysis of process gases used in the semiconductor industry, such as WF_6 , SiH_4 , SiF_4 , and others. These gases are used for chemical vapor deposition (CVD) of tungsten and silicon. The results are essential for the optimization of the process conditions and the reduction of the cost.

The **Inorganic and Coordination Chemistry** section organized two 2–3 h sessions in which a series of graduate students from the various inorganic chemistry departments made short oral presentations concerned with their research activities. In both sessions, the organizers were pleased to note that there was 'standing room only', *i.e.* the lecture theatre was full with interested members of the chemistry community. These two oral programs were followed by a Poster Session containing many dozens of contributions from all of the varied areas of inorganic chemistry. Several of the many excellent posters were chosen for prizes.

The **Organic Chemistry** session was organized as part of the Division of Chemical Research of the fall meeting of the SCS and embraced a total of 26 oral presentations of 15 min. Due to the large number of presentations announced, the assembly was divided into two parallel sessions both interrupted by the common poster session comprising a total of 66 posters. As in previous years, a wide range of topics was covered spanning from analytical, bio-organic and combinatorial topics towards target oriented synthesis and investigations on syn-

thetic methodology including radical chemistry, metal catalysis and photochemistry.

The morning session held in the Montreal room started with a presentation by *Charles-Henry Fabritius* from the group of Prof. Kündig, University of Geneva, on new, so far scarcely known molybdenum-mediated arene transformations. This was followed by an overview and new applications of titanacyclopentene complexes as 1,4-dicarbonyl equivalents provided by *Andreas Goeke*, Givaudan, Dübendorf. The contribution of *Céline Helgen* from the laboratory of Prof. Bochet, University of Geneva, on the synthesis of amides and carbamates by photochemically induced acyl-transfer was succeeded by a discussion of *Adriano F. Indolese*, Rohner AG, Pratteln, on the use of ionic liquids as solvents for metal-catalyzed reactions. The concept of orthogonality in protecting group strategies for solid phase synthesis was presented by *Martin Kessler* from the group of Prof. Giese, University of Basel, using photolabile protecting groups selectively cleavable at different wavelengths. The application of a radical reaction cascade towards the synthesis of deoxy-podophyllotoxin, a precursor of the antimetabolic podophyllotoxin was then presented by *Tanja Kovac* from the group of Prof. Renaud, University of Bern. The morning session was concluded by the talk of *Philipp Krattiger* from the laboratory of Prof. Wennemers, University of Basel on a new concept for the combinatorial search for catalysis.

The Organic Chemistry lectures in the San Francisco room focused mainly on topics with a biological flavor. Contributions were made by groups from the Universities of Zurich, Basel, Geneva, the EPFL-Lausanne, as well as Hoffmann-La Roche Basel. Kicking off the proceedings was a talk from the Schaeferer-group (*Todor Angelov*, University of Zurich) on the intricacies of DNA repair. The synthesis of a series of stably cross-linked nucleotides was described, that are now being used to probe the mechanisms of DNA cross-link repair. Following this, *Matteo Conza* from the Wennemers group (University of Basel) described their ongoing efforts to identify new families of diketopiperazine-based synthetic receptors for peptide ligands. This theme was extended in a later lecture by *Matthias Nold* from the same group, who described the synthesis and application of new templates for diketopiperazine-based receptor design. A fascinating account by *Gopal Das* (Matile group, University of Geneva) recalled the synthesis and properties of new families of β -barrel ion-channel models. These models, based on rigid-rod *p*-octa-

phenyl β -barrels, possess interesting fluorescence properties, and may find potentially valuable applications as sensors. Fluorescence was also a theme in the lecture of *Susanne Gendreizig* (Johnsson group, EPFL) who described their successful efforts to develop methods for labeling specific proteins inside a cell, by utilizing the activity of a DNA-repair enzyme. Applications of this methodology in the area of genomics and proteomics do not seem too far away. Natural products chemistry was at the forefront of the talk by *P. Hebeisen* (Roche) who described the development of inter- and intra-molecular reductive thiolation reactions on aromatic aldehydes. These reactions were key to the successful synthesis of novel DNA gyrase inhibitors based on the natural product cyclothialidine. Finally, *Martin Lochner* (Woggon group, University of Basel) treated his audience to interesting new results on the synthesis and properties of new crown capped porphyrins as cytochrome P450 models. These models are now providing new insights into the structures and properties of the heme coenzyme at the heart of the active site in this important family of redox enzymes.

The afternoon session in the Singapore room was characterized by a broad variety of topics ranging from bioorganic chemistry over the analysis of biosynthetic mechanisms and synthesis to computational chemistry. The broad topic palette was reflected in the internationality of the speakers from Switzerland, Austria and Germany illustrating the recognition of the SCS beyond Switzerland.

The presentation on new insights into the mechanism of the chlorophyll breakdown by *Michael Oberhuber* (research group Prof. Kräutler, University of Innsbruck) was followed by the talk of *Luc Patiny* (EPFL) on new ways for sharing chemical information over the internet. *Petra Tafelmeyer* (research group Prof. Johnsson, EPFL) discussed a new reporter system that allows for monitoring protein-protein interactions. The synthesis of conformationally stable allocolchicinoids was the topic of *Andrei V. Vorogushin's* talk (University of Zürich) and was followed by a presentation on the properties of oligonucleotides that are modified with pyrene by *Hans-Achim Wagenknecht* (TU Munich). The design of enzyme mimetics was the focus of the concluding talk by *Xiao-an Zhang* (research group Prof. Woggon, University of Basel) who presented model compounds for the active site of vanadium haloperoxidase.

About 120 medicinal chemists, a full quarter of their 480 members, gathered in

the lecture hall San Francisco of the Messe Basel to attend the morning and afternoon sessions of **Medicinal Chemistry** within the framework of the fall meeting of the SCS. A record number of 14 short lectures was presented. To accommodate so many speakers we had to limit, for the first time, the presentation time to 15, instead of 20 min. To avoid time-consuming changes of computers, all lectures were stored on one single laptop the day before.

Luigi Calzolari from the group of Nobel Prize winner Prof. Kurt Wüthrich (ETH Zürich) presented the NMR structure of the turtle prion protein, *Marialore Sulpizi* from SISSA (Trieste) Carr-Parinello simulations of the reaction mechanism of caspases, *Christoph Meyer* from the group of Prof. Bernd Giese (University of Basel) showed a novel chemical restriction method, comparable to standard cloning procedures using restriction enzymes.

Katrin Groebke (Roche) presented new and safe anticoagulants, *Suzanne Kolczewski* (Roche) potent, selective and orally active NK1 receptor antagonists, *Eric Vieira* (Roche) positive allosteric modulators of mGluR1 receptors.

Karl-Heinz Altmann (Novartis) showed design and syntheses of highly potent analogs of the naturally occurring antitumor agents Epothilone A and B, *Sylvain Cottens* of transplantation research at Novartis presented statin derivatives as inhibitors of the leukocyte function antigen-1, *René Lattmann* (Novartis) described novel, orally active inhibitors of cathepsin K. *Paul W. Manley* (Novartis) investigates molecular interactions between Glivec and mutant forms of cAbl kinase to overcome the drug resistance problems, *Richard Sedrani* (Novartis) communicated that the spirocyclic subunit of the immunosuppressant natural product Sanglifehrin A can be replaced by structurally simpler moieties and *Gebhard Thoma* (Novartis) showed a novel approach for the control of polyvalent biological interactions.

The two prizes for best oral communications were awarded to *Carlos Garcia-Echeverria* (Novartis) for his presentation on 'Non-Covalent Inhibitors of the 20S Proteasome' and to *Erwin Goetschi* (Roche) for his talk entitled 'From the DNA Gyrase Inhibitor Cyclothialidine to a New Class of Antibacterial Agents'.

In addition, eight posters were presented, three posters from the group of Nauta Prize winner Prof. Bernard Testa (University of Lausanne) prepared by *Veronica Dubbini* (Intramolecular catalysis in the hydrolysis of basic esters), *Corinne Brühlmann* (Dual inhibitors of MAO B and acetylcholinesterase) and *L. Novaroli* (COMT in-

hibitors) and their colleagues, two posters from the group of Prof. Pierre Vogel (University of Lausanne) presented by *Eliazar Rodriguez-Garcia* (Glycosidase inhibitors) and *Sandrine Gerber Lemaire-Audoire* (Selective α -mannosidase inhibitors). *Carsten Spanka* and *Niko Schmiedberg* (Novartis) presented a poster on micro reactors. Finally, two posters were shown by coworkers of Prof. Helmut R. Maecke from the Institute of Nuclear Medicine of the University Hospital Basel, by *M. Ginj* and co-workers on highly potent ligands for somatostatin receptors 2, 3 and 5 and by *Sandrine Fraysse-Phisbien*, who received the poster prize for her contribution on 'Targeted MRI Contrast Agents'.

The meeting on Thursday concluded then with prize ceremonies for the best oral and poster presentations chaired by Wolf Woggon and the presentation of the **Paracelsus Prize** to *Martin Quack* from ETH Zürich by the President André Merbach, 'in recognition of his outstanding theoretical and experimental contributions to the understanding of molecular kinetics'. Martin Quack's Paracelsus prize lecture on 'Molecular Spectra, Reaction Dynamics, Symmetries and Life' gave a broad overview of the research of his group, leading from high resolution molecular spectroscopy to femtosecond and even attosecond dynamics, from fundamental symmetries in high energy particle physics to the selection of biomolecular chirality in life. The prize winning papers and prize lectures will appear in future issues of CHIMIA, we refer to these future papers and the abstracts of the meeting [1] rather than providing any further details here. One thing that has become clear from the fall meeting of the Swiss Chemical Society can be summarized simply: Chemistry is a very alive science – with and without life science.

[1] Fall Meeting 2002 of the Swiss Chemical Society, *Chimia* 2002, 56, 319–418.



Martin Quack and André Merbach