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BridgeVIEW and Chemistry Automation

Olivier Naef*

1. Introduction

This paper discusses how to build an application to control a chemical reactor with BridgeVIEW. The reactor is very simple, but it contains all the features that can be found in an industrial installation controlled by a computer.

The example given in *Fig. 1* is a chemical reactor with a mixer, a temperature indicator, and a level indicator. The reactor has a jacket for controlling the mixture's temperature. It uses steam (from 1 bar to 13 bar) to heat the contents. The temperature of the jacket varies between 100° (212°F) and 180° (356°F). The reactor has two other features:

- 1) We can fill the reactor with water, and a proportional valve adjusts the flow of water into the reactor.
- 2) We can empty the reactor with an on-off valve. A sensor indicates if the valve is really closed.

After the design of the installation, we connect the reactor to the computer with a FieldPoint interface. The application to control this reactor will be written with BridgeVIEW, a graphical programming environment. The application generated is as generic as possible, and as a result, the code can be reused for other industrial automation applications with a minimum amount of modification.

2. Generality

2.1. BridgeVIEW

BridgeVIEW is a graphical programming language for automation application. BridgeVIEW is based on LabVIEW that use the graphical programming language G from *National Instruments*. With BridgeVIEW, you can easily develop Human Machine Interface (HMI) and Supervisory Control and Data Acquisition (SCADA) solutions for manufacturing and process control applications.

For more information, see the Web site: www.natinst.com, or contact *National Instruments Schweiz*, Sonnenberg-

strasse 53, CH-5408 Ennetbaden (Tel. +41 56 200 5151, Fax: +41 56 200 5155, E-Mail: ni.switzerland@natinst.com).

2.2. FieldPoint

FieldPoint is an innovative, modular system with versatile analog and digital I/O capabilities, an unmatched set of usability features, and full suite of software that tightly integrates with LabVIEW, BridgeVIEW, Lookout, and other software packages. You connect the FieldPoint with a serial cable (RS232 or RS485). You can have many (up to 25) stations that are connected to one PC. Each station controls from 1 to 9 I/O modules.

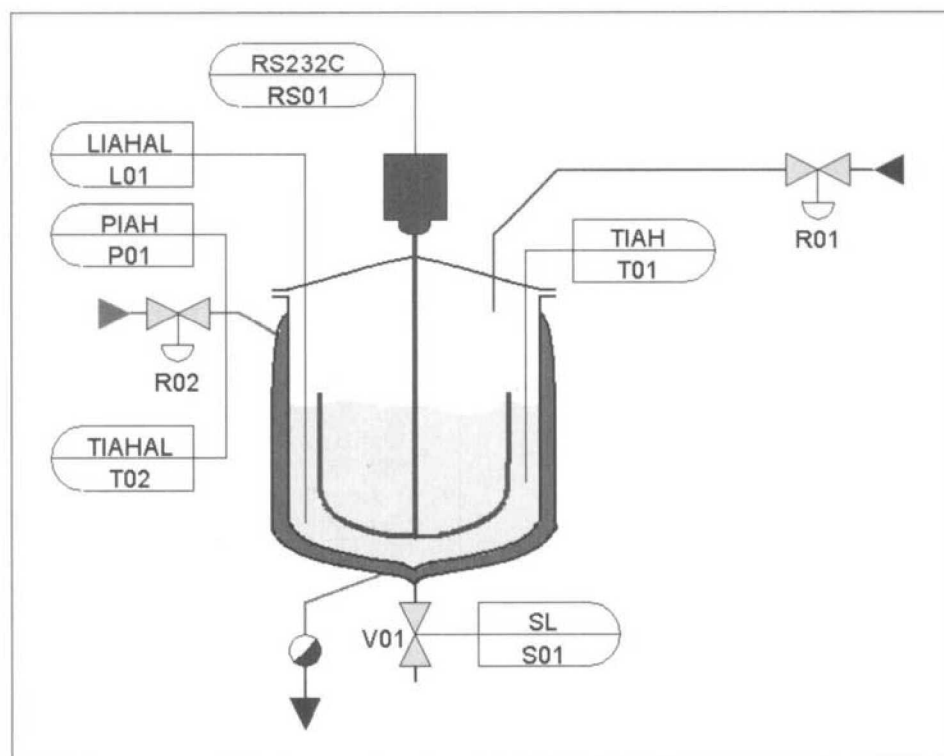


Fig. 1. The simple reactor

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3. HMI

3.1. Introduction

The Human Machine Interface (HMI) is a simplified representation of the installation and an interface for the operator to control and supervise the system (Fig. 2). In an industrial installation, we find many HMIs that represent different aspects of the installation. In an HMI, there is always an active window. From the HMI, we can control the link between the operator and the installation effectively. The operator can work in manual mode (direct access to the elements of the installation or with automation functions) or in batch mode (automatic sequencing of functions to realize a product).

3.2. Main HMI VI

In this system, we have the main HMI VI (the main HMI VI is the primary HMI that controls all the other HMI sub VIs) that represents the global installation and other VIs that provide details on the level system. The main HMI VI starts all other HMI sub VIs. All HMI sub VIs monitor the state of the main HMI and can run only if the main HMI is running. If you close the main HMI VI, all associated VIs will be closed. The main HMI VI can be aborted (abnormal termination) by the main application VI.

3.3. Tags

Another problem addressed is the access rights of the tag. In manual mode, the operator can access the tag to write a value to an actuator. But if the operator starts a function that needs an actuator, the function must disable the write flag of this actuator. The HMI VI can only read the value of the actuator. Hence, the control must be disabled so that the user is not allowed to write to the tag.

4. Simulation

If you have hardware available, this part is not necessary. But, if you don't, it is helpful to have a simulation VI so that you can emulate the installation and see how it will be working in reality. The simulated VI emulates the response of the actuators on the FieldPoint or the simulated FieldPoint and calculates the response from the sensors. All sensors are emulated on the FieldPoint interface with an output (DOT or AOT). The simulation of the reactor's level depends on the proportional input valve and the switch output valve. The closing action of the output is simulat-

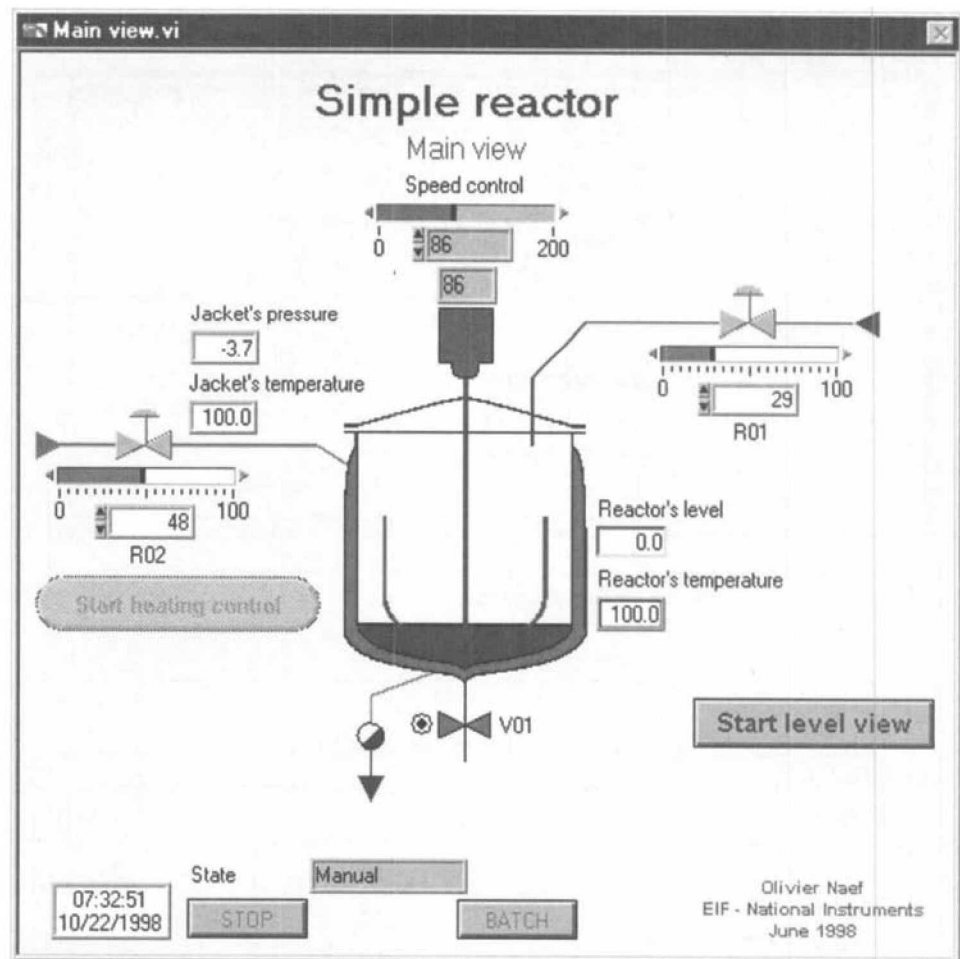


Fig. 2. Main HMI VI

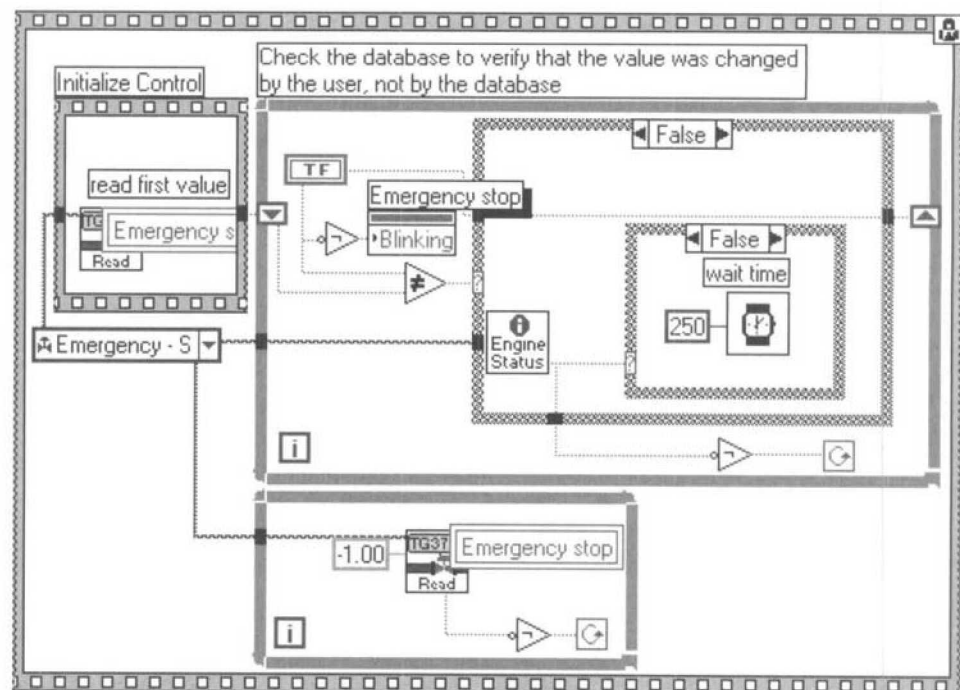


Fig. 3. Write and read tag using the G Wizard

ed with a delay of two seconds. The simulation of the jacket pressure depends on the aperture of the proportional jacket valve. We introduce simulation tools for the jacket pressure: a time shift (delay function) and a time constant (first-order

function). The simulation of the jacket temperature is directly proportional to the pressure. The reactor's temperature is calculated by the Euler's integration of the differential equation for thermal balance.

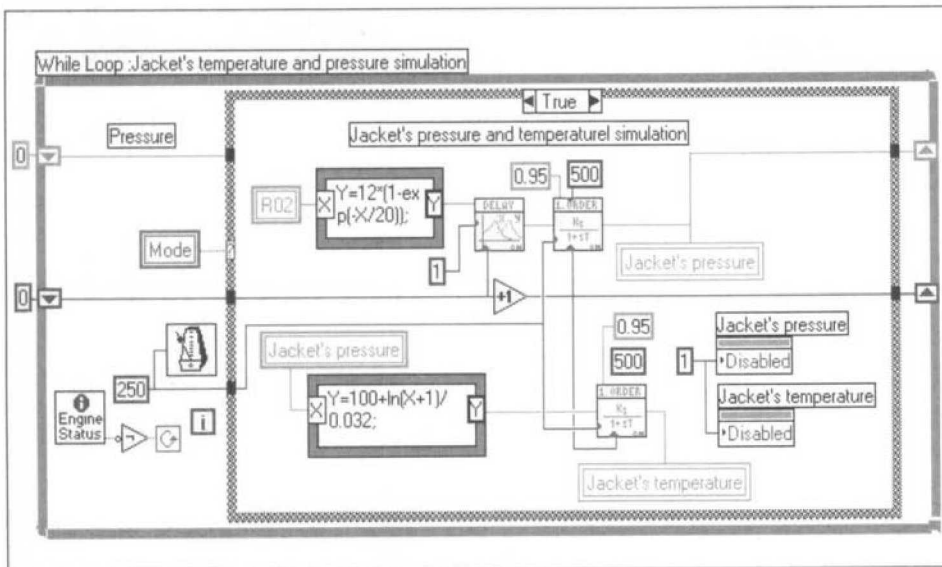


Fig. 4. Jacket's temperature and pressure simulation

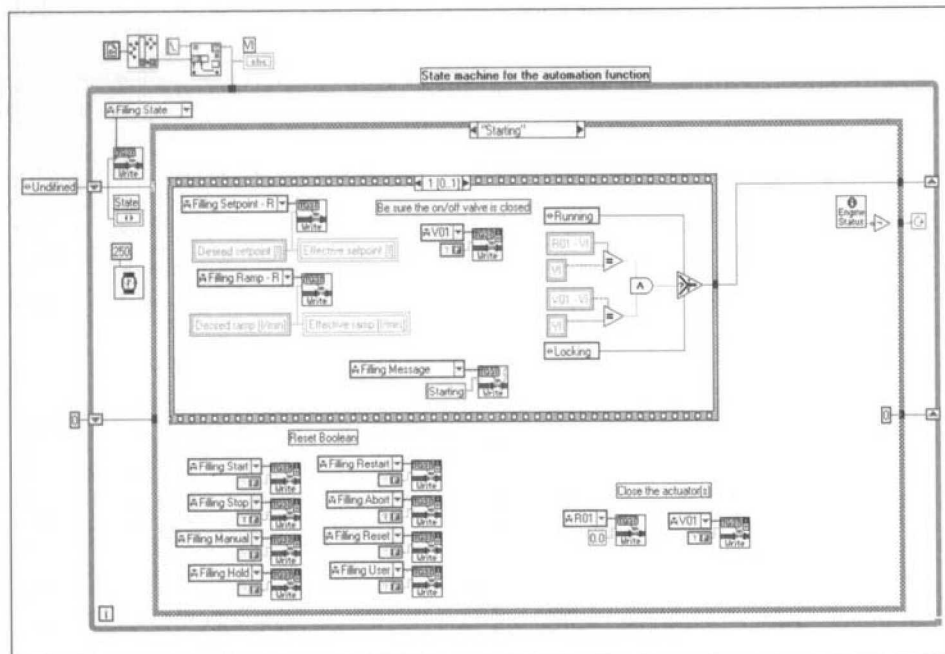


Fig. 5. State machine for the automation function

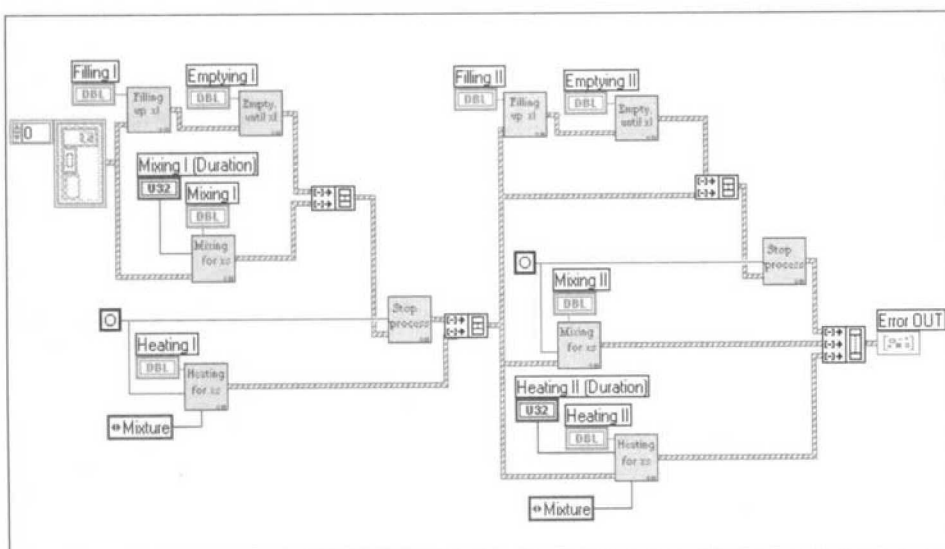


Fig. 6. Batch process VI

The program's structure is parallel loops. For the tag, we use the simple G Wizard that automatically creates the code (Fig. 3). Another example can be seen in Fig. 4 with the loop for the jacket's temperature and pressure simulation.

5. Automation Function

Until this point, we have been running the application in 'manual mode'. We can only write values to actuators and read values from sensors. But you can imagine how difficult it would be to set up an industrial installation without a minimum set of automation functions. In this chemical reactor, the automation function we need is a temperature controller. The temperature controller adjusts the jacket's valve. The operator gives the set point, and the controller works in different modes: reactor's temperature constant, jacket's temperature constant, and a difference between reactor and jacket constant. We build two other automation functions: a filling function and an emptying function. These two functions have an exclusion rule: if you fill the reactor, you cannot empty it at the same time.

The automation function contains two loops: the first loop reads and writes the values to the tags, and the second loop is a state machine that you can see in Fig. 5.

6. Batch

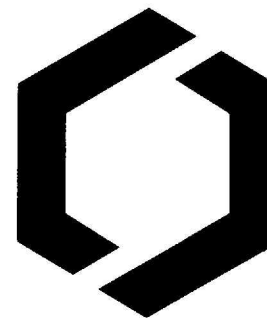
To create a product in a reactor, you can use the automation functions of the installation. If you need to create exactly the same product more than once, the best way is to have the installation runs in an automatic mode. This is called batch processing. Batch processing uses the automation functions. In our example application, we will start with a continuous function: the temperature control (jacket's temperature control). In parallel, we will fill the reactor with water. When the reactor is filled with two liters, we will start the mixer. When it has eight liters, we will stop the introduction of water and change the temperature control (mixture temperature control) for 2 min. After this time, we will stop the temperature control and the mixer. We will then empty the reactor. The batch process is stopped when the emptying function is finished.

The batch uses a main VI to control the batch process, a batch process VI that contains the effective rules of the batch (Fig. 6) and batch functions.

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NSCG

Section of Medicinal Chemistry

Third Swiss School on Medicinal Chemistry, Leysin, October 11–16, 1998

This Course was organised in 1994 for the first time by the Section of Medicinal Chemistry (SMC) of the New Swiss Chemical Society (NSCS) and is held biannually. The 1998 edition was cochaired by Prof. *Bernard Testa* (University of Lausanne) and Prof. *Gerd Folkers* (ETH-Zürich), and it was in fact co-organised by the SMC, the School of Pharmacy of the University of Lausanne and The Department of Pharmacy of the Federal Institute of Technology in Zürich. Such a collaboration between the NSCS and academic departments can only be beneficial and should be encouraged much more vigorously.

The objectives of the Course are to give synthetic chemists, physico-chemists, biochemists and pharmacologists a broad and balanced introduction to the background, concepts and tools of medicinal chemistry, a science at the interface of synthetic organic chemistry, physicochemistry, phytochemistry, biochemistry, pharmacology and toxicology, drug metabolism and disposition, molecular modelling and informatics. Modern preclinical drug research is thus the focus of the Course, which combines dense lectures, tutorials and case studies by experts from university and industry. Active participation was encouraged.

The Course was attended by 70 participants, including 15 Ph.D. students; 16 participants had a Swiss address (*Novartis, Roche, University of Bern, University of Lausanne, Swiss Federal Institute of Technology Lausanne (EPFL) and Zürich (ETHZ)*). On the other hand, 14 participants were coworkers from *Novartis* and 6 from *Roche* (Basel, England, Japan). Indeed, the Course is a very international one. The participants heard 19 lectures, 3 case histories, and had 3 tutorials. The generous contribution of the sponsors *F. Hoffmann-La Roche AG, Novartis AG, Lonza AG* (all Switzerland), *Astra Hässle* (Sweden), *Hoechst Marion Roussel* (France), *Pfizer Central Research* (UK), *Serono Pharmaceutical Research Institute SA* (Switzerland), *SmithKline Beecham Pharmaceuticals* (UK) is warmly acknowledged. It allowed the participation of a relatively large number of Ph.D. students. The Course was again held in Leysin, in the Alpes Vaudoises.

This largely oversubscribed Course stresses the high need of junior medicinal chemists for further education. This task was taken very seriously by the various lecturers making this Course a successful biannual event. The case histories presented by experienced medicinal chemists form an important contribution and illustrate the often forgotten role of serendipity and perseverance in drug discovery.

The Course was opened by some reflections on Medicinal Chemistry by Prof. *Gerd Folkers* (ETH-Zürich). After looking back to older definitions, he cited newer ones taken from the book 'The Practice of Medicinal Chemistry' by Prof. *Camille Wermuth* (University of Strasbourg) and from the 'IUPAC Glossary of Terms Used in Medicinal Chemistry' (see *Ann. Rep. Med. Chem.* **1998**, *33*, 385–395):

'Medicinal Chemistry is a chemistry-based discipline, also involving aspects of biological, medical and pharmaceutical sciences. It is concerned with the invention, discovery, design, identification and preparation of biologically active compounds, the study of their metabolism, the interpretation of their mode of action at the molecular level and the construction of structure-activity relationships'.

Dr. *Richard Ross* (*Novartis*, Basel) described the role of patents, trademarks and how to protect know-how.

Pharmacological assays and parameters were discussed by Prof. *Karl Mohr* (University of Bonn). Via receptor types and radioligand-binding assays, he moved to the up- and downregulation of receptors and modern views on two-state models of 7TM receptors (see below Dr. *S. Hjorth*). In an example using the muscarinic M2 receptor antagonists AF-DX384, and W84 it was demonstrated that some antagonists may not be competitive, but rather bind to an allosteric site.

Prof. *Gilles Paintaud* (University of Tours) gave an introduction to clinical pharmacology, discussing different aspects of phase I–III clinical studies

Dr. *Walter Schilling* (*Novartis*, Basel) gave his view on the target concept in medicinal chemistry. Various families of targets such as enzymes, receptors, intra-cellular and nuclear targets were compared.

Dr. *Siv Hjorth* (University Hospital of Copenhagen) introduced molecular biology in a highly attractive and instructive way. She further reviewed how molecular biology is integrated with medicinal chemistry in today's drug research. As an example, studies on conformational changes in 7TM receptors were discussed. From this collaboration with Prof. *Thue Schwartz* (University Hospital Copenhagen), a number of new binding concepts for agonists and antagonists were developed.

Dr. *René Amstutz* (*Novartis*, Basel) presented the HTS tools used for lead finding. This rapidly expanding and changing field was of keen interest to the audience and demonstrated the impact of partly nonchemical technologies on modern lead finding.

An excellent introduction to combinatorial chemistry was given by PD *Willi Bannwarth* (*Byk Gulden*, Konstanz). It was stressed that in modern discovery strategies, the combination of combinatorial chemistry and HTS heavily relies on a good data management system. Various possibilities using solution- and solid-phase chemistry were discussed. Parallel synthesis of individual compounds was contrasted with the synthesis of complex mixtures that need deconvolution when activity has been found.

How to develop a lead was discussed by Dr. *David Roberts* (*Zeneca*, Macclesfield). He illustrated the process by three examples. The first was a failure story on angiotensin II antagonists, where the key problem was bioavailability. This approach was called a 'fast follow' of a literature/patent lead compound. The second example was based on the clinical candidate ZD1839, which was a chemical follow-up of HTS. The third story was a structure-based design project around DNA gyrase inhibitors. As nicely demonstrated, each of the approaches has strengths and weaknesses and differing resources demands.

In the session on Molecular Design & Lead Optimisation, Dr. *Han van de Waterbeemd* (*Pfizer Central Research*, UK) introduced physicochemical concepts and their role in drug absorption. The basic physicochemical properties were further discussed in a tutorial around the topic Structure-Absorption Relationships.

Prof. *Gerd Folkers* (ETH-Zürich) explained that in molecular modelling studies we look at empirical models, which often can be close to reality. Models can be used to simplify, as a didactical illustration and in mathematical modelling for the simulation of processes. He illustrated his views using the antigen presentation by MHC class I.

Prof. *Hugo Kubinyi* (*BASF*, Ludwigshafen) discussed the impact of computer-assisted lead optimisation on the drug discovery process. He

illustrated how structure-based design was used in a number of projects such as thrombin and HIV inhibitors. Programs like LUDI can be a great help for the generation of ideas. A number of examples also showed the limitation of the idea of molecular similarity and diversity. Very similar compounds sometimes have very different actions.

Various concepts in prodrug design and principles of drug metabolism were reviewed by Prof. *Bernard Testa* (University of Lausanne). He stressed that quantitative predictions in metabolism usually only can be made in structurally related series. The usefulness of expert systems for metabolite prediction was questioned. The pros and cons of prodrugs were discussed. The presentation concluded with some notion about toxification and detoxification processes.

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Dr. *Eric Allémann* (University of Geneva) closed the series of lectures by reviewing a number of current pharmaceutical approaches to drug targeting, including liposomes, nanoparticles and microparticles.

Three two-hour tutorials were presented in interactive sessions by Dr. *David Roberts* (Zeneca, Macclesfield, UK) on Lead Development, by Dr. *Han van de Waterbeemd* (Pfizer, Sandwich, UK) on Structure-Absorption Relationships, and by Dr. *John Comer* and Dr. *Karl Box* (Sirius Analytical Instruments, Forest Row, UK) on the Measurement of pKa and Lipophilicity Profiles by the pH-Metric Method.

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Highly appreciated was the quality of the venue and the informal contact between speakers and participants. Hopefully, the School will be rescheduled for the year 2000.

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Manifestations 1999 – Correction

Thursday
October 14, 1999
Kongresszentrum
Messe Basel

Biotechnology Symposium

organized by:
Dr. *H.G. Leuenberger* on behalf of the NSCS
and the Swiss Coordination Committee for
Biotechnology

Morning:

GENOMICS

Chairman:

Prof. Dr. *P. Philippsen*, Biozentrum Basel

Afternoon:

MOLECULAR DIAGNOSTICS

Chairman: Prof. Dr. *C. Weissmann*,
Universität Zürich

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Chemiepreis der Neuen Schweizerischen Chemischen Gesellschaft

An ihrer Herbstversammlung vom 15. Oktober 1998 in Zürich hat die Neue Schweizerische Chemische Gesellschaft (NSCG) den *Werner-Preis* verliehen. Dieser Preis (CHF 10000.– und Medaille) der NSCG für junge Wissenschaftler ging an Dr. *Thomas R. Ward* vom Departement für Chemie und Biochemie, Universität Bern, in Anerkennung seiner experimentellen und theoretischen Beiträge auf dem Gebiet der Koordinations- und metallorganischen Chemie.

Dr. *Thomas R. Ward* erhält den *Werner-Preis* 1998 für seine hervorragenden Arbeiten auf dem Grenzgebiet von Koordinationschemie und homogener Katalyse. Dr. *Ward* verknüpft in seiner Forschung mit grossem Erfolg quantenchemische Konzepte und Berechnungen mit synthetischer Chemie. Mit dem zielgerichteten Aufbau einer komplexen



H.L. Senti (Präsident NSCG)

T.R. Ward (Preisträger)

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Wintgens, David, 2000 Neuchâtel

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Division, Biotechnology Department, PRNB,
Bldg. 62/213, CH-4070 Basel
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Chemiepreis der Neuen Schweizerischen Chemischen Gesellschaft

An ihrer Herbstversammlung vom 15. Oktober 1998 in Zürich hat die Neue Schweizerische Chemische Gesellschaft (NSCG) den *Werner-Preis* verliehen. Dieser Preis (CHF 10000.– und Medaille) der NSCG für junge Wissenschaftler ging an Dr. *Thomas R. Ward* vom Departement für Chemie und Biochemie, Universität Bern, in Anerkennung seiner experimentellen und theoretischen Beiträge auf dem Gebiet der Koordinations- und metallorganischen Chemie.

Dr. *Thomas R. Ward* erhält den *Werner-Preis* 1998 für seine hervorragenden Arbeiten auf dem Grenzgebiet von Koordinationschemie und homogener Katalyse. Dr. *Ward* verknüpft in seiner Forschung mit grossem Erfolg quantenchemische Konzepte und Berechnungen mit synthetischer Chemie. Mit dem zielgerichteten Aufbau einer komplexen



H.L. Senti (Präsident NSCG)

T.R. Ward (Preisträger)

Eisenverbindung mit Stickstoff- und Sauerstoff-Kavitäten gelang ihm die Herstellung eines über den Redoxvorgang betriebenen molekularen Schalters. Eingehende Studien dynamischer Prozesse metallorganischer Moleküle befassen sich mit der enantioselektiven Katalyse. Die

theoretisch untermauerten, zielorientierten synthetischen Arbeiten von Dr. *Ward* liefern einen bedeutenden Beitrag zur Erforschung neuartiger Metallkomplexe mit spezifischer Funktionalität, ein Gebiet mit grossem Potential, auch in der angewandten Forschung.

Neue Mitglieder

Biland, Andreas, 4055 Basel
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Fokas, Christian, 8055 Zürich
Forster, Andrea, 4310 Rheinfelden
Heckel, Alexander, 8044 Zürich
Hennessy, Brian, 3012 Bern
Jucker, Walter, Dr.,
4310 Rheinfelden
Künzle, Niklaus, 9500 Wil
Lelais, Gérald, 6943 Vezia
Rippert, Andreas, Dr.,
8330 Pfäffikon
Walczak, Maciej A.,
60-801 Poznan (Polen)
Widmer, Hans, Dr., 4125 Riehen
Wintgens, David, 2000 Neuchâtel
Zürcher, Fabio, Dr., 8052 Zürich

illustrated how structure-based design was used in a number of projects such as thrombin and HIV inhibitors. Programs like LUDI can be a great help for the generation of ideas. A number of examples also showed the limitation of the idea of molecular similarity and diversity. Very similar compounds sometimes have very different actions.

Various concepts in prodrug design and principles of drug metabolism were reviewed by Prof. *Bernard Testa* (University of Lausanne). He stressed that quantitative predictions in metabolism usually only can be made in structurally related series. The usefulness of expert systems for metabolite prediction was questioned. The pros and cons of prodrugs were discussed. The presentation concluded with some notion about toxification and detoxification processes.

The basic principles of pharmacokinetics were treated by Prof. *Luc Balant* (University of Geneva). Furthermore, metabolic variability during drug development as a potential source of problems was discussed.

The question how to study drug absorption and distribution was addressed by Dr. *Alessandro Probst* (Novartis, Basel). He summarised ideas about theoretical considerations as well as *in vitro* and *in vivo* (*in situ*) methods.

Dr. *Eric Allémann* (University of Geneva) closed the series of lectures by reviewing a number of current pharmaceutical approaches to drug targeting, including liposomes, nanoparticles and microparticles.

Three two-hour tutorials were presented in interactive sessions by Dr. *David Roberts* (Zeneca, Macclesfield, UK) on Lead Development, by Dr. *Han van de Waterbeemd* (Pfizer, Sandwich, UK) on Structure-Absorption Relationships, and by Dr. *John Comer* and Dr. *Karl Box* (Sirius Analytical Instruments, Forest Row, UK) on the Measurement of pKa and Lipophilicity Profiles by the pH-Metric Method.

Highlights of the School were three case histories of recently introduced drugs. The fascinating story of the discovery of the lipase inhibitor tetrahydrolipstatin (Orlistat, Xenical) was presented by Dr. *Pierre Barbier* (Roche, Basel). The total synthesis of this compound goes back to 1983, while its marketing only started in 1998. Dr. *Peter Bühlmyer* (Novartis, Basel) gave an insight how the angiotensin II antagonist valsartan was discovered from the lead DuP-753 or losartan. Dr. *Nick Terrett* (Pfizer, UK) described how sildenafil (Viagra) was found from a PDE project originally aiming at the treatment of cardiovascular diseases such as hypertension and angina. Since the reported erections by healthy volunteers in early clinical studies in 1992, the program was focused on male erectile dysfunction, resulting in the introduction of Viagra in 1998.

Highly appreciated was the quality of the venue and the informal contact between speakers and participants. Hopefully, the School will be rescheduled for the year 2000.

Dr. *Han van de Waterbeemd*

Pfizer Central Research, Dept. Drug Metabolism
Sandwich, Kent CT13 9NJ, UK

Tel.: +44 1304 646179, Fax: +44 1304 656433

E-Mail: han_waterbeemd@sandwich.pfizer.com

Manifestations 1999 – Correction

Thursday
October 14, 1999
Kongresszentrum
Messe Basel

Biotechnology Symposium

organized by:
Dr. *H.G. Leuenberger* on behalf of the NSCS
and the Swiss Coordination Committee for
Biotechnology

Morning:

GENOMICS

Chairman:

Prof. Dr. *P. Philippsen*, Biozentrum Basel

Afternoon:

MOLECULAR DIAGNOSTICS

Chairman: Prof. Dr. *C. Weissmann*,
Universität Zürich

Information:

Dr. *H.G. Leuenberger*

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INFORMATION



Bringing IUPAC up to date^{a)}

John Jost*

Is an organisation formed in the aftermath of World War I still relevant to the needs of the 21st century? Most chemists are familiar with the name IUPAC from their first course in organic chemistry, where they studied IUPAC nomenclature for the first, and perhaps last time. A somewhat smaller number know that IUPAC is the International Union of Pure and Applied Chemistry. For those chemists whose familiarity with the organisation does not go much beyond this, the question naturally arises: what's left for IUPAC to do?

One thing is the standardisation of nomenclature, terminology, symbols, procedures and data. All of this is vital, but often goes unnoticed by practitioners who are unaware of how the process works.

The need to validate data for use in models and equations of state becomes more crucial as more data are produced and individual chemists have less time to examine the provenance of the data in published data sets. And the language of chemistry must change as the science develops. As in any other language, there is a need to accommodate slang and neologisms, but also to uphold the rules of grammar and the meanings of words. One of IUPAC's core activities is the publication of a series of guides to the nomenclature of chemistry.

But IUPAC does much more than develop recommendations on nomenclature, terminology and evaluated data. Each year, it sponsors more than 20 international symposia in most areas of chemistry, and a biennial congress that focuses on newly developing fields in the chemical sciences.

It also organises CHEMRAWN (Chemical Research Applied to

World Needs) conferences in areas of socio-political importance. It contributes to advances in methods for teaching chemistry, especially in developing countries. Its committee on chemistry and industry sponsors conferences and workshops on topics of interest to industry, such as chemical plant safety.

IUPAC's mission is to 'advance the worldwide aspects of the chemical sciences and to contribute to the application of chemistry in the service of mankind'. In doing this, IUPAC promotes the norms, values, standards and ethics of science, and advocates the free exchange of scientific information and unimpeded access of scientists to participation in activities related to the chemical sciences.

However, as with many international organisations that work through volunteers, IUPAC has been criticised as being too slow, too rigid and dominated by the members of a 'charmed circle'. These criticisms have been voiced in one way or another for 40 years, but have been more publicly expressed in the past decade. The sentiment expressed is that chemistry has changed but IUPAC has not.

IUPAC has responded by re-examining the basic purposes of the union and the way in which its scientific work is organised. It has set up the strategy development and implementation committee, comprising IUPAC officers and prominent chemists from outside IUPAC.

This committee has developed a strategic plan and recommended a new management process for IUPAC's scientific work. Assuming its recommendations are adopted in general, if not in detail, then IUPAC will have responded to the three criticisms cited above in a decisive manner.

The new management of the union's scientific work will be centred in seven broadly constituted division committees, rather than in 37 'permanent' commissions. This addresses the issue of a rigid structure by converting the working part

of the union from commissions with long-term members to working groups with a membership assembled for the duration of the project.

This also addresses the charmed circle issue. The need to create working groups for each new project will encourage outreach to chemists worldwide. The short-term nature of the commitment to a working group will encourage young scientists and those in industry to devote time to IUPAC without the need to make the long-term commitment that membership on a commission implies.

The timeliness question will be addressed in two ways. The first is by defining projects in terms of goals and time limits. It is expected that most projects will take about two years from approval to completion. The necessary corollary to this is the funding of projects at a level necessary to allow completion in the planned time. By devoting more resources to fewer projects, those projects should be completed more quickly and the results will be more useful to practising chemists.

These proposed changes assume that there are many chemists who would be willing to participate in IUPAC activities given the opportunity. The organisation is opening itself to the global chemical community. All chemists are considered potential participants in IUPAC projects. By encouraging input from all chemists, IUPAC expects to receive more project ideas in areas of interest to industry and society.

The union will be relying on electronic communication to involve more chemists in its work. I invite all of you to visit our web site (<http://www.iupac.org>) to see what IUPAC is doing now and to revisit it regularly to see what it will be doing in the future.

But more than visiting, I invite you to participate. Let us know what you think are the important issues in your area of chemistry. The success of IUPAC depends on the willingness of chemists around the world to take part in its activities. If the planned changes result in more participation, then they will have been successful.



Federation of European Chemical Societies

Appointment of New President Elect of FECS Dr. Reto Battaglia

At its recent General Assembly, FECS appointed Dr. *Reto Battaglia* of the New Swiss Chemical Society, as its President Elect. *Reto Battaglia* will serve one year as President Elect before succeeding Prof. *Lauri Niinisto* as President of FECS after the 1999 General Assembly in Helsinki on September 16–17.

Reto Battaglia has been involved in the work of the Federation since 1981, having been a member of and, since 1995, Chairman of the Division of Food Chemistry. He has been President of the Swiss Society of Food and Environmental Chemistry and has been active in the IUPAC Commission on Food Chemistry.

Following his doctoral studies at ETH-Zürich, *Reto Battaglia* was a

post-doctoral fellow at the University of Manchester (UK) in organic synthetic chemistry. In 1973, he joined the Cantonal Laboratory of Zürich, later becoming deputy head. Since 1989 he has been Director of *Migros Laboratories*, Zürich.

Note: The Federation of European Chemical Societies is a voluntary association, the object of which is to promote cooperation in Europe between those non-profit-making scientific and technical societies in the field of chemistry whose membership consists largely of individual qualified chemists and whose interests include the science and/or practice of chemistry. It was founded in 1970.

* Dr. Jost is executive director of IUPAC, based in Research Triangle Park, North Carolina, USA.

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News

**A New COST Chemistry Action:
'New Molecules towards Human Health Care'**

Five COST Chemistry Actions were initiated the last two years covering: Chemistry of Metals in Medicine (D8: ending 29.4.2001), Advanced Computational Chemistry of Increasingly Complex Systems (D9: 18.5.2002), Innovative Methods and Techniques for Chemical Transformations (D10: 18.5.2002), Supramolecular Chemistry (D11: 14.1.2003), Organic Transformations, Selective Processes and Asymmetric Catalysis (D12: 17.12.2002). These areas of research are now complemented by the new COST Action D13 in the field of bioactive molecules: 'New molecules towards human health care'.

Objectives

The main objective of the Action D13 is binding together established sciences of chemistry, biochemistry, biology and pharmacology. The action should develop knowledge on the relationships between the molecular structure and the biological activity of synthetic and naturally occurring compounds. It will promote know-how and understanding of the interactions between molecules and biological processes which are relevant in maintaining and restoring human health. The projects in this action will contribute to the scientific knowledge base essential for academic and industrial pharmaceutical and medical research. The action will stimulate the establishment of European research networks and it will bring related projects closer together and, by doing so, stimulate and strengthen them.

Why a COST Action in this Field?

As a result of the fact that every year more biological processes can be described in terms of molecules and molecular interactions, the importance of bioorganic studies for understanding health problems and drug development is steadily increasing. The application of new techniques and methods in human health-care research, like genomics or combinatorial sciences, requires more and more interdisciplinary work. In view of the scope of the field, international cooperations between academic groups and contacts with appropriate R&D groups of industries are of vital importance. Although every research group in the field of bioorganic chemistry or pharmaco-chemistry has its own international contacts, the action will contribute to a broader platform for discussions, which is essential for a successful multidisciplinary approach.

Status

The COST Action D13 has been launched for a five-years period finishing 22.9.2003. The Swiss groups from the academia and industry can participate according to the rules given on the COST web site: <http://www.unil.ch/cost/chem/>. For more details, contact in Switzerland:

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E-Mail: hanspeter.schelling@group.novartis.com

Konferenz der Schweizerischen Wissenschaftlichen Akademien (CASS): Neuer Präsident

Die Konferenz der Schweizerischen Wissenschaftlichen Akademien (CASS) hat einen neuen Präsidenten: *Bernard Hauck*, Präsident der Schweizerischen Akademie der Naturwissenschaften (SANW) und Professor für Astrophysik an der Universität Lausanne. *Hauck* löst auf den 1. Januar 1999 *Carl Pfaff*, alt Präsident der Schweizerischen Akademie der Geistes- und Sozialwissenschaften (SAGW), ab.

Die CASS vereint die Akademien der Geistes- und Sozialwissenschaften, der medizinischen Wissenschaften, der technischen Wissenschaften sowie der Naturwissenschaften. Sie dient der Koordination und Reflexion zu Fragen, welche Wissenschaft und Gesellschaft beschäftigen. Sie fördert Aktivitäten im Rahmen von Kommissionen, z.B. der Kommission für Forschungspartner-schaften mit Entwicklungsländern

(KFPE). Als Stimme der wissenschaftlichen Gemeinde der Schweiz äussert sich die CASS zu Fragen der Wissenschaftspolitik, organisiert Fachgespräche unter Teilnahme internationaler ExpertInnen und publiziert deren Ergebnisse.

Die wichtigsten Gesprächspartner der CASS auf nationaler Ebene sind der Schweizerische National-

fonds (SNF), der Schweizerische Wissenschaftsrat (SWR), das Bundesamt für Bildung und Wissenschaft (BBW) und die Gruppe für Wissenschaft und Forschung (GWF). Die CASS steht aber auch in Verbindung mit internationalen Einrichtungen wie European Science Foundation und Convention of All European Academies.

Exxon Chemical European Science and Engineering Award 1999

Exxon Chemical Europe wishes to increase the interaction between its technical community and European Universities and Research Institutions through its 'European Science and Engineering Programme' (ESEP).

As part of this programme, ESEP is issuing a biennial award in various domains of chemical research.

This award, amounting to 40000 ECU, will be granted in 1999 to support fundamental or applied research in the field of 'Oxygenates from Carbon Monoxide'.

On behalf of *Exxon Chemical*, the 'Fonds voor Wetenschappelijk On-

derzoek - Vlaanderen' will grant the 1999 Award.

Applications have to be sent to the Secretariaat Generaal of the 'Fonds voor Wetenschappelijk Onderzoek - Vlaanderen' before June 15, 1999.

More detailed information and application forms can be obtained from:

Fonds voor Wetenschappelijk Onderzoek - Vlaanderen
Secretariaat Generaal
Egmontstraat 5
B-1000 Brussel
Tel.: +32 2 512 91 10
Fax: +32 2 512 58 90

Novartis Completes Acquisition of Fermentation Plant from HMR

Basel/Kundl, November 2, 1998 - *Novartis* announced today that *Biochemie GmbH*, its Austria-based pharmaceutical generics unit, has completed the acquisition of the Frankfurt fermentation plant of *Hoechst Marion Roussel Germany GmbH*. The deal, first announced in February, extends *Biochemie's* product range and further strengthens its leading position as one of the world's largest manufacturers of bulk antibiotics. Financial details were not disclosed.

The Frankfurt site is a biotech production unit that manufactures fermentation products, such as penicillin, and intermediates for other antibiotics. With an annual turnover

in the region of 120 million CHF, it has a similar fermentation capacity to *Biochemie's* Kundl plant.

Biochemie has agreed to take over ca. 350 employees working in the 'fermentation group' from HMR by 1999. No redundancies are envisaged with this acquisition.

Biochemie GmbH is a biotechnology company with operations throughout the world and is one of the largest manufacturers of oral and sterile penicillins. With a staff of 1883, *Biochemie* is Austria's biggest pharmaceutical manufacturer and exporter. *Biochemie* belongs to the Generics Sector of *Novartis*, which generated sales of 1.5 billion CHF in 1997.

New Transplantation Drug *Simulect*® Granted European Approval**Novartis further strengthens its leadership in transplantation medicine**

Basel, October 16, 1998 - *Novartis* announced today that the European Commission has granted marketing approval in the EU for *Simulect*® (basiliximab) for the prevention of acute rejection episodes in kidney transplant recipients. *Simulect* will be the first drug of its

kind to become available in the EU in the coming months.

Dr. *Jerry Karabelas*, Head of *Novartis Healthcare* and CEO of *Novartis Pharma* commented: '*Simulect* is designed to complement *Novartis'* flagship product *Neoral*®, one of the most widely used medications in transplantation. *Simulect* reduces the risk of graft rejection without increasing the level of side

effects. It has already been launched successfully in the USA and in Switzerland and will further strengthen our leadership position in transplantation medicine'.

Simulect is a monoclonal antibody that enhances the immunosuppressive effect of *Neoral*. Because of its high, specific affinity for the cells that attack the transplant in the rejection process, only two doses of

Simulect are required: one before and the other a few days after transplantation. This simple dosing schedule means that patients do not have to return to hospital for further antibody treatments after they have been discharged, avoiding both inconvenience and further costs. Patients are being followed closely to assess the effect of *Simulect* on improving long-term graft survival.

Tagungen, Veranstaltungen, Weiterbildung

PhandTA 4 4th Symposium/Workshops on Pharmacy and Thermal Analysis

March 23–26, 1999, University of Karlsruhe, Germany

eurostar (European Society for Thermal Analysis, Calorimetry, Thermodynamics, and Chemical Reactivity): <http://www.eurostar-science.org>

Information:

Dr. E. Marti

Novartis Service AG

K-127.5.80

CH-4002 Basel

Tel.: +41 61 696 53 48/696 45 64

Fax: +41 61 696 93 04

E-Mail: niklaus.martin@sn.novartis.com

Vorträge

Novartis Chemistry Lectureship 1998/1999

Mittwoch, 10.30 Uhr
Auditorium Horburg, K-430.3.20
Müllheimerstrasse, Basel

- | | |
|-----------------|--|
| 13. Januar 1999 | Prof. S.D. Rychnovsky
UC Irvine, USA
'Structure and Reactivity of Anion, Cation and Radical Intermediates in 1,3-Dioxane Rings: Applications to Total Synthesis' |
| 3. Februar 1999 | Prof. M. Lautens
University of Toronto, Canada
'New Catalytic Asymmetric Reactions and Their Application to the Synthesis of Bioactive Compounds' |

Berner Chemische Gesellschaft

Mittwoch, 16.30 Uhr
Hörsaal EG 16, Departement für Chemie und Biochemie
Freiestrasse 3, Bern
(Kaffee um 16.10 Uhr vor dem Hörsaal)

- | | |
|----------------|--|
| 6. Januar 1999 | Prof. J. Simon
ESPCI, Laboratoire de Chimie Inorganique et Electrochimie des Matériaux Moléculaires, Paris Cedex, France
'A Few Aspects of Supramolecular Engineering' |
|----------------|--|

- | | |
|-----------------|---|
| 13. Januar 1999 | Prof. R. Huber
Max-Planck-Institut für Biochemie, Abteilung Strukturforchung, Planegg-Martensried, Deutschland
'Proteine und ihre Strukturen am Schnittpunkt von Chemie, Physik und Biologie' |
| 3. Februar 1999 | Dr. C. Kleiber
Gruppe für Wissenschaft und Forschung, Eidg. Departement des Innern, Bern
'Pour l'université' |

Freiburger Chemische Gesellschaft

Dienstag, 17.15 Uhr
Grosser Hörsaal der Chemie-Institute
der Universität (Pérolles)

- | | |
|-----------------|---|
| 5. Januar 1999 | Prof. K. Bernauer
Chimie de Coordination et Chimie Bioinorganique, Université de Neuchâtel
'Chiral Metal Complexes as Probes in Electrotransfer Reactions Involving Native or Mutant Recombinant Metalloproteins' |
| 26. Januar 1999 | Prof. K. Hostettmann
Institut de Pharmacognosie et Phytochimie, Université de Lausanne
'The Potential of Plants as Source of New Drugs' |

Société Chimique de Genève

Lundi, 17.30 h
Uni Sciences II
Quai Ernest-Ansermet, Genève

- | | |
|-----------------|--|
| 18. Januar 1999 | Dr. C. Piguet
Université de Genève
'Chimie supramoléculaire des lanthanides: Entre tradition et nouveauté' |
| 8. Februar 1999 | Prof. O. Kahn
Institut de Physique des Solides, Bordeaux, France
'Hystérésis et effet mémoire en chimie moléculaire' |

Biochemische Institute der Universität Zürich

Donnerstag, 17.00 Uhr
Winterthurerstrasse 190
Zürich-Irchel, Hörsaal 85

- | | |
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| 7. Januar 1999 | Dr. S. Raina
Centre Médicale Universitaire, Département de Biochimie Médicale, Université de Genève
'Protein Folding in the Periplasm of <i>Escherichia coli</i> ' |
| 14. Januar 1999 | Prof. U. Baumann
Departement Chemie/Biochemie, Universität Bern
Titel folgt |
| 21. Januar 1999 | Prof. K. Basler
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'Organizers and Cell Affinities in <i>Drosophila</i> ' |
| 28. Januar 1999 | Dr. R. Eckner
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'p300 anmd CBP in Growth Control and Differentiation' |

effects. It has already been launched successfully in the USA and in Switzerland and will further strengthen our leadership position in transplantation medicine'.

Simulect is a monoclonal antibody that enhances the immunosuppressive effect of *Neoral*. Because of its high, specific affinity for the cells that attack the transplant in the rejection process, only two doses of

Simulect are required: one before and the other a few days after transplantation. This simple dosing schedule means that patients do not have to return to hospital for further antibody treatments after they have been discharged, avoiding both inconvenience and further costs. Patients are being followed closely to assess the effect of *Simulect* on improving long-term graft survival.

Tagungen, Veranstaltungen, Weiterbildung

PhandTA 4 4th Symposium/Workshops on Pharmacy and Thermal Analysis

March 23–26, 1999, University of Karlsruhe, Germany

eurostar (European Society for Thermal Analysis, Calorimetry, Thermodynamics, and Chemical Reactivity): <http://www.eurostar-science.org>

Information:

Dr. E. Marti

Novartis Service AG

K-127.5.80

CH-4002 Basel

Tel.: +41 61 696 53 48/696 45 64

Fax: +41 61 696 93 04

E-Mail: niklaus.martin@sn.novartis.com

Vorträge

Novartis Chemistry Lectureship 1998/1999

Mittwoch, 10.30 Uhr
Auditorium Horburg, K-430.3.20
Müllheimerstrasse, Basel

- | | |
|-----------------|--|
| 13. Januar 1999 | Prof. S.D. Rychnovsky
UC Irvine, USA
'Structure and Reactivity of Anion, Cation and Radical Intermediates in 1,3-Dioxane Rings: Applications to Total Synthesis' |
| 3. Februar 1999 | Prof. M. Lautens
University of Toronto, Canada
'New Catalytic Asymmetric Reactions and Their Application to the Synthesis of Bioactive Compounds' |

Berner Chemische Gesellschaft

Mittwoch, 16.30 Uhr
Hörsaal EG 16, Departement für Chemie und Biochemie
Freiestrasse 3, Bern
(Kaffee um 16.10 Uhr vor dem Hörsaal)

- | | |
|----------------|--|
| 6. Januar 1999 | Prof. J. Simon
ESPCI, Laboratoire de Chimie Inorganique et Electrochimie des Matériaux Moléculaires, Paris Cedex, France
'A Few Aspects of Supramolecular Engineering' |
|----------------|--|

- | | |
|-----------------|---|
| 13. Januar 1999 | Prof. R. Huber
Max-Planck-Institut für Biochemie, Abteilung Strukturforchung, Planegg-Martensried, Deutschland
'Proteine und ihre Strukturen am Schnittpunkt von Chemie, Physik und Biologie' |
| 3. Februar 1999 | Dr. C. Kleiber
Gruppe für Wissenschaft und Forschung, Eidg. Departement des Innern, Bern
'Pour l'université' |

Freiburger Chemische Gesellschaft

Dienstag, 17.15 Uhr
Grosser Hörsaal der Chemie-Institute
der Universität (Pérolles)

- | | |
|-----------------|---|
| 5. Januar 1999 | Prof. K. Bernauer
Chimie de Coordination et Chimie Bioinorganique, Université de Neuchâtel
'Chiral Metal Complexes as Probes in Electrotransfer Reactions Involving Native or Mutant Recombinant Metalloproteins' |
| 26. Januar 1999 | Prof. K. Hostettmann
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Anorganisch-chemisches Institut der Universität Zürich

17.00 Uhr

Seminarraum 34 F 48

Winterthurerstrasse 190, Zürich-Irchel

5. Januar 1999

Dienstag

Dipl.-Chem. *D. Rattat*

Anorganisch-chemisches Institut der Universität Zürich

'Synthese und Reaktivität der komplexchemischen d⁶Tc(I)- und Re(I)-Dicarbonyl-Nitrosyl-Baugruppen – auf dem Weg zu neuen Radiopharmaka'

6. Januar 1999

Mittwoch

Dipl.-Chem. *M. Wagner*

Anorganisch-chemisches Institut der Universität Zürich

'Chemie am Seegrund'

7. Januar 1999

Donnerstag

Dipl.-Chem. *D. Unseld*

Anorganisch-chemisches Institut der Universität Zürich

'σ-Alkynyl-Mangan-Komplexe – Design, Synthese und strukturelle Eigenschaften von 'Kohlenstoffstangen' mit paramagnetischen Baugruppen'

8. Januar 1999

Freitag

Dipl.-Chem. *P. Ott*

Anorganisch-chemisches Institut der Universität Zürich

'Herstellung und Charakterisierung von Au-, Cu-, Te-Schichten'

15. Januar 1999

Freitag

Prof. Dr. *R. Nesper*

Laboratorium für Anorganische Chemie, ETH-Zürich

'Die Welt der Siliciumcluster'

20. Januar 1999

Mittwoch

Dipl.-Chem. *B. Krebs*

Anorganisch-chemisches Institut der Universität Zürich

'Synthese und Charakterisierung von Vanadium-Heteropolyanionen und deren Bedeutung bei der Oxidation von Ammoniak'

29. Januar 1999

Freitag

Dr. *A. Hafner**Ciba* Catalyst Research, Research Centre Marly
'Katalyse bei *Ciba SC* – einige ausgewählte Beispiele'

5. Februar 1999

Freitag

Prof. Dr. *L. Dahlenburg*

Institut für Anorganische Chemie, Universität Erlangen, Deutschland

'Neues aus der Synthese- und Koordinationschemie chiraler und achiraler Phosphorliganden mit P,P- und P,X-Donorsätzen'

Chemische Gesellschaft Zürich

Mittwoch, 17.15 Uhr

Hörsaal CAB D2, ETH-Zentrum, Chemiegebäude

Universitätstrasse 6, Zürich

20. Januar 1999

Prof. Dr. *P. Kinnunen*

Department of Medical Chemistry, University of Helsinki, Helsinki, Finland

'Biomembranes as Supramolecular Assemblies: A Lipid Point of View'

27. Januar 1999

Prof. Dr. *T.M. Kutchan*

Laboratorium für Molekulare Biologie, Universität München, Deutschland

'Gene Technology with Natural Products: How Far Are We? What Is Still to Come?'

3. Februar 1999

Prof. Dr. *H.E. Gaub*

Ludwig-Maximilian-Universität, München, Deutschland

'Mechanical Experiments with Individual Molecules – Nanophysics Meets Molecular Biology'

Organisch-chemisches Institut der Universität Zürich

Dienstag, 17.15 Uhr

Hörsaal 91

Winterthurerstrasse 190

Zürich-Irchel

5. Januar 1999

Dr. h.c. *R. Kaiser**Givaudan-Roure Research Ltd.*, Dübendorf

'Vom Duft der Pflanzen. Biologische, chemische und olfaktorische Aspekte'

12. Januar 1999

Prof. Dr. *P. Rüedi*

Organisch-chemisches Institut, Universität Zürich

'Stereochemie der Inhibition von Serien-Hydrolasen mit Organophosphaten'

19. Januar 1999

J. Heerklotz (Gruppe *Hesse*)

Organisch-chemisches Institut, Universität Zürich

'Synthesen neuer Cyclophane durch Ringerweiterungsreaktionen'

26. Januar 1999

Prof. Dr. *B. Giese*

Institut für Organische Chemie, Universität Basel

'Stereochemie und Memory Effekt in der Radikalchemie'

2. Februar 1999

Institutsangehörige

Organisch-chemisches Institut, Universität Zürich

Posterpräsentationen

Laboratorium für Technische Chemie der ETH-Zürich**Sicherheit und Umweltschutz in der Chemie**

Freitag, 10.15 Uhr

Seminarraum CAB D 43

Universitätstrasse 6, Zürich

8. Januar 1999

Dr. *H. Belevi*

Stoffhaushalt und Entsorgungstechnik, EAWAG

'Bestimmung und Aussagekraft von Transferkoeffizienten in Kehrlichtverbrennungsanlagen'

15. Januar 1999

Dr. *M. Thüer**Ciba SC AG*, Pratteln

'Technische Lösungen für den Umweltschutz in der Industrie: Was kann eine wissenschaftliche Ausbildung dazu beitragen?'

22. Januar 1999

Dr. *T. Wiedmann*

Akademie für Technikfolgenabschätzung in Baden-Württemberg, Stuttgart, Deutschland

'Regionale Nachhaltigkeit im Spannungsfeld globaler Veränderungen: Relevanz von Umweltindikatoren'

29. Januar 1999

Dr. *J. Krüger**Celanese GmbH*, Frankfurt, Deutschland'Wandel einer EHS-Organisation beim Übergang zu dezentralen Firmenstrukturen am Beispiel *Hoechst AG* – *Celanese*'

5. Februar 1999

Vorstellung der Diplomarbeiten

Einladung folgt zu einem späteren Zeitpunkt

Laboratorium für Organische Chemie der ETH-Zürich

Montag, 16.30 Uhr
Hörsaal CHN A 31
Universitätstrasse 16, Zürich

11. Januar 1999 Prof. *M. Mann*
Odense University, Denmark
'Applications of MALDI and Nano-electrospray in Protein Microcharacterization'
18. Januar 1999 Prof. *V.K. Aggarwal*
University of Sheffield, UK
'Catalytic Asymmetric Epoxidation and Related Reactions'
1. Februar 1999 Prof. *A. Alexakis*
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'Asymmetric Conjugate Addition of Organocopper Reagents'

Kompetenzzentrum Analytische Chemie CEAC-ETHZ

<http://www.ceac.ethz.ch>

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'Recent Trends in Trace Element Determination and Speciation Using Chromatographic Techniques in Combination with Inductively Coupled Plasma Mass Spectrometry'

Neue Bücher**Buchbesprechung: Analytical Chemistry**

Edited by R. Kellner, J.-M. Mermet, M. Otto, H.M. Widmer
Verlag Wiley-VCH, 1998, 916 Seiten, ISBN 3-527-28881-3

Das lang erwartete Werk ist erschienen. Die Lektüre macht Spass. Was lange währt, wird endlich gut!

Der Untertitel des Werkes 'The Approved Text to the FECS Curriculum Analytical Chemistry' deutet bereits auf ein Lehrbuch von besonderer Bedeutung. Die Ursprünge des Werkes gehen auf Arbeiten der 'Working Party in Analytical Chemistry' (heute Division of Analytical Chemistry) der FECS 1990-1992 zurück. Die Erkenntnis, dass die analytisch-chemische Ausbildung europaweit vernachlässigt worden war, verbessert und auf einen gemeinsamen hohen Standard gebracht

werden müsse, um den Anforderungen eines offenen, qualitätsbewussten Europas zu genügen, war auslösendes Moment für die Schaffung eines analytischen EUROCURRICULUMs mit dem dazu gehörenden, nun vorliegenden Lehrbuch.

In fünf grossen Abschnitten: 1. General Topics, 2. Chemical Analysis, 3. Physical Analysis, 4. Computer-Based Analytical Chemistry, 5. Total Analysis Systems präsentieren die 30 Autoren aus 14 Ländern die analytische Chemie auf dem neuesten wissenschaftlichen Stand. Von besonderem Wert sind die Kapitel, in denen die Anwendung und

Bedeutung der analytischen Chemie in Technologie und in der Wirtschaft dargestellt wird.

Die Behandlung der Techniken und Methoden in fast enzyklopädischem Umfang gestattet nicht nur dem Studierenden eine Vertiefung und gleichzeitig einen raschen Überblick. Auch Chemiker und Naturwissenschaftler in der Praxis werden den Text zur Wissensauffrischung nutzen können. Nicht nur das. Mit der umfassenden wissenschaftlichen Darstellung, gekoppelt mit Themen von technisch-wirtschaftlicher Bedeutung, ist es auch gelungen, ein Nachschlagewerk zu schaffen. Ein kleiner Kritikpunkt ist hier anzubringen: das Inhaltsverzeichnis ist angesichts der Informationsfülle kurz, z.B. fehlt der wichtige Begriff 'measurement uncertainty'.

Das Werk beginnt mit der Bedeutung der analytischen Chemie und Darstellung der Analyse als Arbeitsprozess der Problemlösung. Mit der kritischen Auseinandersetzung mit Fehlerquellen und Messungenauigkeit wird auch klar gemacht, dass es bei der analytischen Chemie mehr als um blosses Datengenerieren geht. Damit wird auch die Wichtigkeit der Datenqualität in der analytischen Chemie selber, aber auch deren Rolle in der industriellen Qualitätssicherung (Qualitätskontrolle, Zertifizierung, Akkreditierung) eindrücklich beschrieben. Die vielen Hinweise auf Primärliteratur erleichtern den raschen Einstieg in die Materie.

Hoch anzurechnen ist den Herausgebern und Autoren, dass auch modernste Entwicklungen berücksichtigt und kompetent beschrieben wurden. Beispielsweise sind Abschnitte über Techniken der Rastermikroskopie (STM, AFM), Kapillarenzonelektrophorese, matrixunterstützte Laserdesorptionen- und -ionisations- (MALDI) Massenspektrometrie, miniaturisierte Totalanalytensysteme oder Biosensorik vorhanden. Auch etwas exotischere Methoden wie die Field Flow Fractionation (FFF) fehlen nicht.

Aus didaktischer Sicht ist das Werk hervorragend als Ergänzung

zum Analytik-Unterricht oder zum Selbststudium geeignet, da es übersichtlich gegliedert und sehr vollständig ist. Die enorme Fülle macht es aber dem Studierenden nicht leicht, Gewichtungen vorzunehmen und neueste Entwicklungen herauszuschälen und zu verfolgen.

Die vielen Grafiken, Figuren und Tabellen eignen sich für den Unterricht; die Qualität der Figuren sind aber sehr uneinheitlich; z.T. sehr klein (z.B. in Kapitel 8.2) oder schlecht reproduziert (z.B. Fig. 9.2-15). Eine CD-ROM-Version des Textes oder der Figuren und Tabellen würde einen Transfer auf andere im Unterricht gebräuchliche Datenträger erleichtern.

Die 'Fragen und Probleme' am Ende jeden Kapitels sind etwas einfach, und nach genauem Studium des Textes beinahe trivial zu beantworten. Sie können allenfalls als Anregung für Prüfungsaufgaben dienen. Für das Selbststudium des Buches jedoch könnte der Leser von besser gestellten Fragen und einem dazugehörigen Antwort-Teil profitieren. Für den Studierenden wären Aufgaben mit Lösungen eine willkommene Hilfe zum Selbststudium, entsprechend den vorangestellten 'learning objectives' und den guten 'worked examples'.

Die (englische) Sprache ist klar und verständlich. Obwohl heute von jedem Chemiestudierenden erwartet wird, dass Englisch als Fachsprache beherrscht und akzeptiert wird, stellt sich die Frage, ob Übersetzungen in andere Sprachen wünschbar sind.

Der Preis ist angesichts des Werkes angemessen, auch für Studierende.

Insgesamt ein überzeugendes Werk, dem man eine grosse Verbreitung wünscht. Damit es als Lehrbuch und Nachschlagewerk lebt, wird ein stetiges updating und upgrading notwendig sein. In diesem Sinne ist zu hoffen, dass die Verwerter dieses Buches ihre Anregungen für kommende Auflagen machen werden.

P.R. Radvila, M. Schär, R. Zenobi

Bei der Redaktion eingetroffene Bücher

P. Blümler, B. Blülich, R. Botto, E. Fukushima (Eds.)
'Spatially Resolved Magnetic Resonance'
Wiley-VCH, 1998

R. Steudel
'Chemie der Nichtmetalle', 2. vollständig neu bearbeitete Auflage
Walter de Gruyter, 1998

C. Janiak, T.M. Klapötke, H.-J. Meyer
'Moderne Anorganische Chemie', Ed. E. Riedel
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Die Behandlung der Techniken und Methoden in fast enzyklopädischem Umfang gestattet nicht nur dem Studierenden eine Vertiefung und gleichzeitig einen raschen Überblick. Auch Chemiker und Naturwissenschaftler in der Praxis werden den Text zur Wissensauffrischung nutzen können. Nicht nur das. Mit der umfassenden wissenschaftlichen Darstellung, gekoppelt mit Themen von technisch-wirtschaftlicher Bedeutung, ist es auch gelungen, ein Nachschlagewerk zu schaffen. Ein kleiner Kritikpunkt ist hier anzubringen: das Inhaltsverzeichnis ist angesichts der Informationsfülle kurz, z.B. fehlt der wichtige Begriff 'measurement uncertainty'.

Das Werk beginnt mit der Bedeutung der analytischen Chemie und Darstellung der Analyse als Arbeitsprozess der Problemlösung. Mit der kritischen Auseinandersetzung mit Fehlerquellen und Messungenauigkeit wird auch klar gemacht, dass es bei der analytischen Chemie mehr als um blosses Datengenerieren geht. Damit wird auch die Wichtigkeit der Datenqualität in der analytischen Chemie selber, aber auch deren Rolle in der industriellen Qualitätssicherung (Qualitätskontrolle, Zertifizierung, Akkreditierung) eindrücklich beschrieben. Die vielen Hinweise auf Primärliteratur erleichtern den raschen Einstieg in die Materie.

Hoch anzurechnen ist den Herausgebern und Autoren, dass auch modernste Entwicklungen berücksichtigt und kompetent beschrieben wurden. Beispielsweise sind Abschnitte über Techniken der Rastermikroskopie (STM, AFM), Kapillarenzonelektrophorese, matrixunterstützte Laserdesorptionen- und -ionisations- (MALDI) Massenspektrometrie, miniaturisierte Totalanalytensysteme oder Biosensorik vorhanden. Auch etwas exotischere Methoden wie die Field Flow Fractionation (FFF) fehlen nicht.

Aus didaktischer Sicht ist das Werk hervorragend als Ergänzung

zum Analytik-Unterricht oder zum Selbststudium geeignet, da es übersichtlich gegliedert und sehr vollständig ist. Die enorme Fülle macht es aber dem Studierenden nicht leicht, Gewichtungen vorzunehmen und neueste Entwicklungen herauszuschälen und zu verfolgen.

Die vielen Grafiken, Figuren und Tabellen eignen sich für den Unterricht; die Qualität der Figuren sind aber sehr uneinheitlich; z.T. sehr klein (z.B. in Kapitel 8.2) oder schlecht reproduziert (z.B. Fig. 9.2-15). Eine CD-ROM-Version des Textes oder der Figuren und Tabellen würde einen Transfer auf andere im Unterricht gebräuchliche Datenträger erleichtern.

Die 'Fragen und Probleme' am Ende jeden Kapitels sind etwas einfach, und nach genauem Studium des Textes beinahe trivial zu beantworten. Sie können allenfalls als Anregung für Prüfungsaufgaben dienen. Für das Selbststudium des Buches jedoch könnte der Leser von besser gestellten Fragen und einem dazugehörigen Antwort-Teil profitieren. Für den Studierenden wären Aufgaben mit Lösungen eine willkommene Hilfe zum Selbststudium, entsprechend den vorangestellten 'learning objectives' und den guten 'worked examples'.

Die (englische) Sprache ist klar und verständlich. Obwohl heute von jedem Chemiestudierenden erwartet wird, dass Englisch als Fachsprache beherrscht und akzeptiert wird, stellt sich die Frage, ob Übersetzungen in andere Sprachen wünschbar sind.

Der Preis ist angesichts des Werkes angemessen, auch für Studierende.

Insgesamt ein überzeugendes Werk, dem man eine grosse Verbreitung wünscht. Damit es als Lehrbuch und Nachschlagewerk lebt, wird ein stetiges updating und upgrading notwendig sein. In diesem Sinne ist zu hoffen, dass die Verwerter dieses Buches ihre Anregungen für kommende Auflagen machen werden.

P.R. Radvila, M. Schär, R. Zenobi

Bei der Redaktion eingetroffene Bücher

P. Blümler, B. Blülich, R. Botto, E. Fukushima (Eds.)
'Spatially Resolved Magnetic Resonance'
Wiley-VCH, 1998

R. Steudel
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Walter de Gruyter, 1998

C. Janiak, T.M. Klapötke, H.-J. Meyer
'Moderne Anorganische Chemie', Ed. E. Riedel
Walter de Gruyter, 1999