Johann Gasteiger − Germany's Pioneer in Chemoinformatics

Johann Gasteiger—known to his colleagues and friends as "Johnny"—was born on October 27, 1941 in Dachau, Germany. Between 1961 and 1967, he studied chemistry at the Ludwig-Maximilians-University of Munich, at the Swiss Federal Institute of Technology (ETH), and also at the University of Zurich (Switzerland). Johann graduated in Organic Chemistry under Professor Rolf Huisgen from the Ludwig-Maximilians-University of Munich and then in 1971 received his doctorate, specializing in "Mechanism of Reactions of Cyclo-octatetraene". After a postdoctoral fellowship in quantum chemistry between 1971 and 1972 with Prof. Andrew Streitwieser, Jr. at the University of California in Berkeley (U.S.A.), investigating "ab initio Calculations on Carbanions", Johnny returned to Germany and taught at the Technical University of Munich (TUM) until 1993. During this time, he worked together with Prof. I. Ugi as a scientific assistant and completed his habilitation in 1979, specializing in the area of "Chemical Reactions and Reactivity − Models and Algorithms". Johnny was appointed a Professor at the TUM in 1988.

Because of his broad expertise in the field of coding chemical reactions, Johann became consultant to the Beilstein Institute, Frankfurt am Main, and from 1987 to 1991 he was project manager for the development of the ChemInformRX reaction database for FIZ CHEMIE in Berlin, Germany. Following the retirement of the managing director, Christian Weiske in 1993, the directorship of the FIZ Chemie Berlin was offered to Johann, which he graciously declined, favoring his beloved academic research.

Between 1985 and 1989, Johann chaired the working party "Computers in Chemistry", a division of "Chemie-Information-Computer" (CIC) of the German Chemical Society. Later, he became a member of the board and chairman of the CIC. He was also appointed to the vice-chairmanship of the European working party "Computational Chemistry" of the Federation of European Chemical Societies (FECS) in 1986, a post that he held until as recently as 2004.

In 1994, Johann moved from Munich to the University of Erlangen-Nuremberg where he cofounded the "Computer-Chemie-Centrum" (CCC) together with Professors Paul von Ragué Schleyer and Tim Clark. Together, they were the protagonists in the development of the CCC that became a world-leading institution in the field of computational chemistry and chemoinformatics. In this field alone, Johnny has authored more than 300 scientific publications. He is considered not only as one of the founders of the field but also as an enthusiastic advocate of chemoinformatics and computational chemistry in Germany.

Throughout his career, his guiding theme and main research interest has been the development of software to solve problems in drug design and chemical reactivity. His research has concentrated on the searching and optimization of lead structures for drug discovery and drug design, the simulation of chemical reactions, organic synthesis design, knowledge extraction from reaction databases, an analysis of biochemical pathways, the simulation of spectra, and chemical information processing by neural networks and genetic algorithms. Collaborations with Mario Marsili (Università di l' Aquila, Italy) and Professor Jure Zupan (Minister of Higher Education, Science and Technology, Republic of Slovenia) have resulted in numerous publications.

At the beginning of his career, Johann's seminal research group in Munich included Clemens Jochum and Mario Marsili whose interests were not only the pursuit of computer chemistry techniques applied to reactions but also the problem of pursuing in-depth chemical discussions with a reactive stoichiometry of Weisswurst and Hefe-Weissbier, the local Bavarian delicacies. Later Clemens Jochum was responsible for the design and development of the electronic version of the *Beilstein Handbook of Organic Chemistry*, the Beilstein Database, a project for which Johann provided his knowledge as a consultant.

From the very beginning, the major interest of the research group was understanding chemical reactions and the development of methods for modeling and storing chemical reaction and reaction mechanism data. The development

10.1021/ci600240w CCC: $33.50
Published on Web 10/21/2006

resulted in three systems: **EROS** (Elaboration of Reactions for Organic Synthesis) for the simulation and prediction of organic reactions, **WODCA** (Workbench for the Organization of Data for Chemical Applications) for the design of organic syntheses initially developed by Wolf-Dietrich Ihlenfeldt, and **CORA** (Classification of Organic Reactions for Applications) for the derivation of knowledge on chemical reactions from reaction databases, developed by Lingran Chen and Oliver Sacher.

The ability to distribute chemical software (chemical information systems) and databases (structure and reaction databases) generated with this software was finally realized in 1989 by Johann, Heinz Saller, and Peter Löw, who founded the software company ChemoData, a predecessor of InfoChem. Additionally, Wolf-D. Ihlenfeldt developed the **CACTVS**−System that today still provides tools for processing chemical structures, reactions, and spectra. The NCI-database, available free of charge, was also produced with this software. The recent evolution of a chemoinformatics system is now the **MOSES** (MOlecular Structure Encoding System) project, a molecular chemical data toolkit designed and developed by Achim Herwig, Thomas Kleinöder, and several other members of the group.

Many technologies evolved from Johann's research group. An automatic three-dimensional structure generator **CORINA** (COoRdINAtes) was developed by Jens Sadowski building on prior work in the group by Christian Hiller and Christine Rudolph.[1] The physicochemical effects and properties that are implicated in the breaking and making of bonds in organic reactions were consolidated into the software package **PETRA** (Parameter Estimation for the Treatment of Reactivity Applications) that also includes the PEOE (Partial Equalization of Orbital Electronegativities) method.

The PEOE method for calculating charges, also known as the Gasteiger−Marsili charges, is now incorporated in practically all molecular software packages. The PEOE method is probably the most cited paper of the group,[2] although this manuscript had been rejected three times.

During the last 15 years Johann has moved into inductive learning methods as a central theme of his research, to address the multidimensionality of chemical information. In 1993 Johnny published, together with Jure Zupan, a book about *Neural Networks in Chemistry* which was so successful that it found a second edition in 1999.[3] With neural networks, Johann and his research group have been successful in predicting the relationships between chemical structure and biological activity, in modeling chemical reactivity, in comparing combinatorial libraries, identifying bonding in synthesis design, modeling the relationships between chemical structure and spectra, enriching reaction databases, and exploring many other problems in chemistry.

One of the most recent projects has seen a significant contribution to systems biology. By transforming the information from "Biochemical Pathways", the poster originally produced by Boehringer Mannheim (now Roche), into an interactive metabolic reaction database, biochemists can explore endogenous cellular metabolism in detail.

Johann's research group was always large and often consisted of approximately 20 chemists, biologists, and computer scientists, financed from diverse international funding bodies. He has been a source of inspiration to many of his colleagues.

Due to his continuing success in developing chemical software, it was only a question of time before Johann founded a spin-off company from the Computer-Chemie-Centrum at the University of Erlangen-Nuremberg. Since 1997, Molecular Networks GmbH (www.mol-net.com) has provided multifaceted, innovative software to the chemical, biotechnology, and pharmaceutical industries.

As previously mentioned, Johann has always promoted chemoinformatics by giving introductory lectures in this field. Information describing all the tools developed in his group is freely accessible in the online services on the Web (http://www2.chemie.uni-erlangen.de). There you may also find a great deal of the (German) teaching material, developed for a multimedia project (VS-C) under the management of FIZ CHEMIE Berlin.

Last but not least, a mention must be made of the highly successful *Handbook and Textbook of Chemoinformatics*, published in 2003, which gives a very comprehensive overview of this field.[4,5]

In recognition of his work Johann has received many awards, e.g. in 1991 he was awarded with the Gmelin-Beilstein Medal of the German Chemical Society for Achievements in Computer Chemistry. In 1997, he received the Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society for advancing computerization of chemistry in areas of artificial intelligence, neural networks, chemical reactions, 3D databases, and structure−activity relationships. The recognition continued in 2005 when Johann received the Mike Lynch Award from the Chemical Structure Association and the ACS Award for Computers in Chemical and Pharmaceutical Research in 2006.

Professor Dr. "Johnny" Gasteiger will become emeritus in April 2007, after a long and successful career. Now a new life will start, and his other interests including his family, hobbies, and, of course, his company will provide a lively retirement.

Thanks for everything Johnny!

REFERENCES AND NOTES

(1) Gasteiger, J.; Marsili, M. Iterative partial equalization of orbital electronegativity: a rapid access to atomic charges. *Tetrahedron* **1980**, *35* (22), 3219−3222.

(2) Sadowski, J.; Gasteiger, J.; Klebe, G. Comparison of Automatic Three-Dimensional Model Builders Using 639 X-ray Structures. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1000−1008.

(3) Zupan, J.; Gasteiger, J. *Neural Networks in Chemistry and Drug Design*, 2nd ed.; Wiley-VCH: Weinheim, 1999; 380 pp.

(4) *Chemoinformatics − A Textbook*; Gasteiger, J., Engel, T., Eds.; Wiley-VCH: Weinheim, Germany, 2003; 650 pp.

(5) *Handbook of Chemoinformatics − From Data to Knowledge*; Gasteiger, J., Ed.; Wiley-VCH: Weinheim, 2003; Vol. 4, 1870 pp.

Thomas Engel*

Chemical Computing Group AG
Kaiser-Wilhelm-Ring 11
50672 Cologne, Germany

CI600240W