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Contributors

Jan H. Noordik received his M.Sc. in Chemistry from Groningen University and his Ph.D. in Crystallography from Nijmegen University in 1971. Following a faculty position in Crystallography at the University of Nijmegen, a postdoctoral fellowship with Prof. Jeffrey at Brookhaven National Laboratory in 1975, another faculty position in Nijmegen, and a sabbatical year at the University of Colorado at Boulder in 1984, he co-founded the CAOS/CAMM Center (the Dutch national academic center for cheminformatics and bioinformatics, now called the Centre for Molecular and Biomolecular Informatics, or CMBI) in 1985. From 1986 up to his retirement in 2001 he was the director of this institute. His research interests include(d) X-ray crystallographic structure determination, molecular modeling, and the use of computerized chemical data storage and retrieval techniques (nowadays called cheminformatics) to further chemical research and education. He is the (co-) author of dozens of articles in scientific journals in these fields.

Hens Borkent received his Ph.D. in organic chemistry from the University of Amsterdam in 1976.

Following a postdoctoral fellowship at the University of Nijmegen, and a faculty position at the University of Dar es Salaam, Tanzania, he joined the CAOS/CAMM Center (now the Centre for Molecular and Biomolecular Informatics, or CMBI) at the University of Nijmegen in 1986. His scientific interests include computational organic chemistry and visualization in teaching of chemistry.

Tim Clark was born in southern England and studied chemistry at the University of Kent at Canterbury, where he was awarded a first class honors Bachelor of Science degree in 1969. He obtained his Ph.D. from the Queen's University, Belfast, in 1973 after working on the thermochemistry and solid phase properties of adamantane and diamantane derivatives. After two years as an Imperial Chemical Industries Postdoctoral Fellow in Belfast he moved to Princeton University as a NATO Postdoctoral Fellow working for Paul Schleyer in 1975. He then followed Schleyer to the Institut für Organische Chemie of the Universität Erlangen-Nürnberg in 1976. He is currently Technical Director of the Computer-Chemie-Centrum in Erlangen. His research areas include the development and application of quantum mechanical methods in inorganic, organic, and biological chemistry, electron transfer theory, and the simulation of organic and inorganic reaction mechanisms. He is the author of 200 articles in scientific journals and two books and is the editor of the Journal of Molecular Modeling.

Dave Fletcher obtained a degree in chemistry from Oxford University in the mid 1980s, staying on to complete a D.Phil. in High-Resolution Molecular Spectroscopy.

Three years of postdoctoral research followed at Arizona State University before he joined the newly-expanded U.K. Chemical Database Service in 1993 to support the spectroscopic area. Since then he has driven much of the technological development of the Service, particularly interface design and the integration of different datasets.

Johann (**Johnny**) **Gasteiger** studied chemistry at the Universities of Munich and Zurich. He stayed at the University of California in Berkeley and taught at the Technical University of Munich. In 1994 he co-founded the Computer-Chemie-Centrum at the University of Erlangen. He is one of the founders of chemoinformatics in Germany and has produced more than 200 scientific publications in this field. Johnny was a consultant to the Beilstein Institute and to FIZ CHEMIE Berlin, where he was the project manager for the development of the ChemInformRX reaction database. He was awarded the Gmelin-Beilstein Medal of the German Chemical Society and the Herman Skolnik Award of the American Chemical Society.

Jan Kelder obtained his Ph.D. in Chemistry from the University of Amsterdam in 1974 in the group of Prof. Hans Cerfontain. In the same year he joined the Analytical Chemistry Department at Organon, Oss, the Netherlands, as Research Scientist, to study quantitative structure-property and quantitative structure-activity relationships. He currently holds the position of Research Associate in the Molecular Design & Informatics Department. His research interests have centered on quantitative structure-activity relationships, molecular modeling, computational ADME, property predictions, and combinatorial library design.

Frank Leusen studied Pharmacy and Bio-Pharmaceutical Sciences at Leiden University and received his Ph.D. from Nijmegen University in 1993. He worked as a research consultant for Novartis AG in Switzerland before joining Accelrys Ltd (formerly Molecular Simulations Ltd) in Cambridge, U.K., in 1993. While there he founded and directed the Pharmaceutical Development Consortium, an international partnership with industrial members and academic advisors dedicated to advancing the state-of-the-art in the simulation of the organic solid state. In 2003 he joined the newly-founded Institute of Pharmaceutical Innovation at Bradford University, U.K., where he holds the position of Senior Scientist. His current research interests include crystal structure prediction from first principles, prediction of organic solid state properties, and simulation of crystal nucleation.

Bob McMeeking obtained his first and Ph.D. degrees in Chemistry from the University of Bristol. He moved on to pursue his postdoctoral research in the area of ligand field theory at Cambridge and at the Australian National University, with Malcolm Gerloch and Ray Martin respectively. He then worked at the Cambridge Crystallographic Data Centre for a period of just over a year. This inspired him to continue his developing interest in chemical database systems. He moved to the Chemical Database Service at Daresbury in 1984 and has remained there ever since.

Sam Motherwell is a Ph.D. graduate of St Andrews University (1967) in organic chemical crystallography. He joined the Cambridge Crystallographic Data Centre (CCDC) in 1968 where he developed the first versions of the substructure search software, analysis of 3D-geometric fragments, and the Pluto graphics program. In 1978 he joined Cambridge University Library where he developed the on-line catalog system. He returned to the CCDC in 1992 as Research Manager, whereby he is responsible for research in areas of chemistry making use of the database information, particularly crystal structure prediction, H bonding, and crystal engineering.

Martin Ott received his M.Sc. in Chemistry (Organic Chemistry and Computer Science) from the University of Groningen, and his Ph.D. in Chemistry (Computer-Assisted Organic Synthesis) from the University of Nijmegen. Since 1985 he has been manager of cheminformatics services and research at the CAOS/CAMM Center, now the Centre for Molecular and Biomolecular Informatics (CMBI), at the University of Nijmegen. His research interests focus on the application of computers in organic chemistry, especially synthesis and structure representation.

Marco Timmers did his graduate research on nucleic acid and carbohydrate chemistry in the group of Professor Jacques van Boom at Leiden University in the Netherlands and received his Ph.D. in Bio-Organic Chemistry in 1996. He then joined Organon's Medicinal Chemistry Department and became involved in various research projects in the areas of immunology, atherothrombosis, and reproductive medicine. In 2001 he was appointed Associate Director of the Medicinal Chemistry Department and since 2002 he has held the position of Project Leader Lead Optimization Profertility.

Paul Verwer received both his M.Sc. and Ph.D. from Utrecht University, the Netherlands. After holding postdoctoral positions at NV Organon and the CAOS/CAMM Center, he currently holds the position of Project Leader at the Laboratory of Solid State Chemistry at the University of Nijmegen. His research interests focus on computer simulations of crystalline systems and include simulations of crystal growth, morphology, polymorphism, and organic epitaxy.

Markus Wagener graduated in Chemistry from the Technical University, Munich, in 1988 and received his Ph.D. degree in 1993 under the guidance of Prof. J. Gasteiger. In 1994 he moved with Prof. Gasteiger to the Computer-Chemie-Centrum in Erlangen. After a postdoctoral stay at SmithKline Beecham in King of Prussia, from 1996 to 1997, he joined the Department of Molecular Design & Informatics at Organon in Oss. His research interests include novel data analysis techniques and how they can be applied to small molecule drug design.