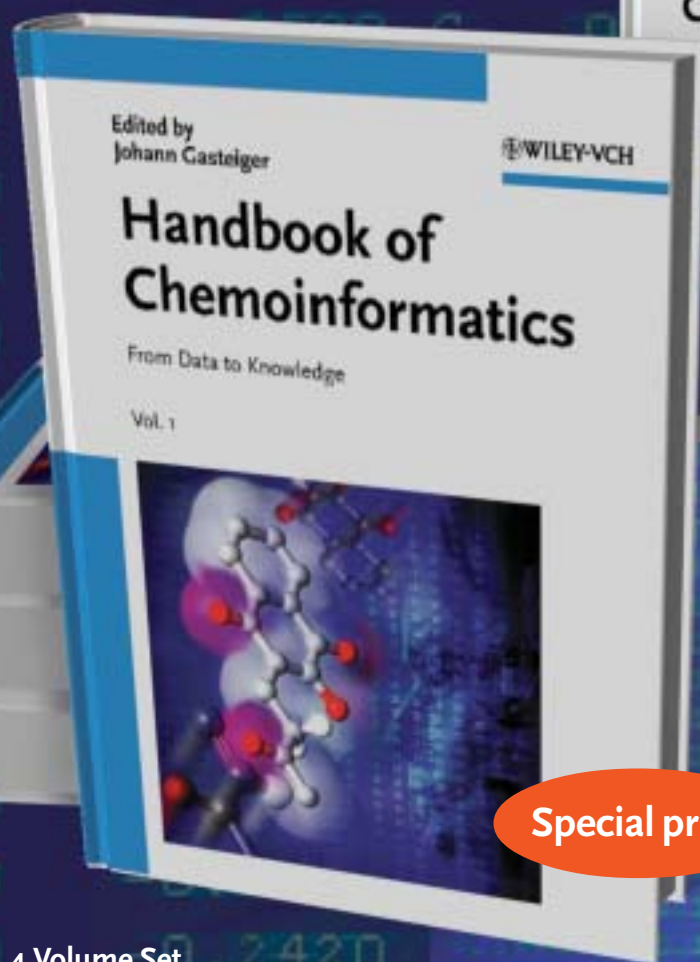


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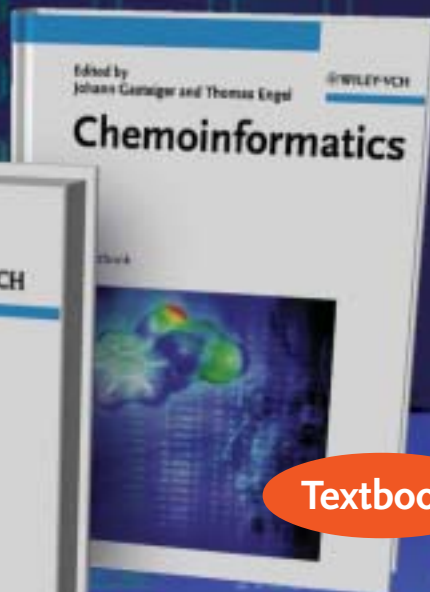


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Gasteiger, J. / Engel, T. (eds.)  
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- Methods for Data Analysis
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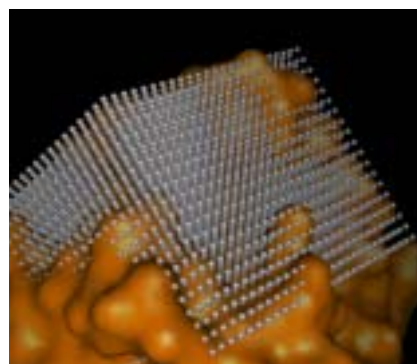
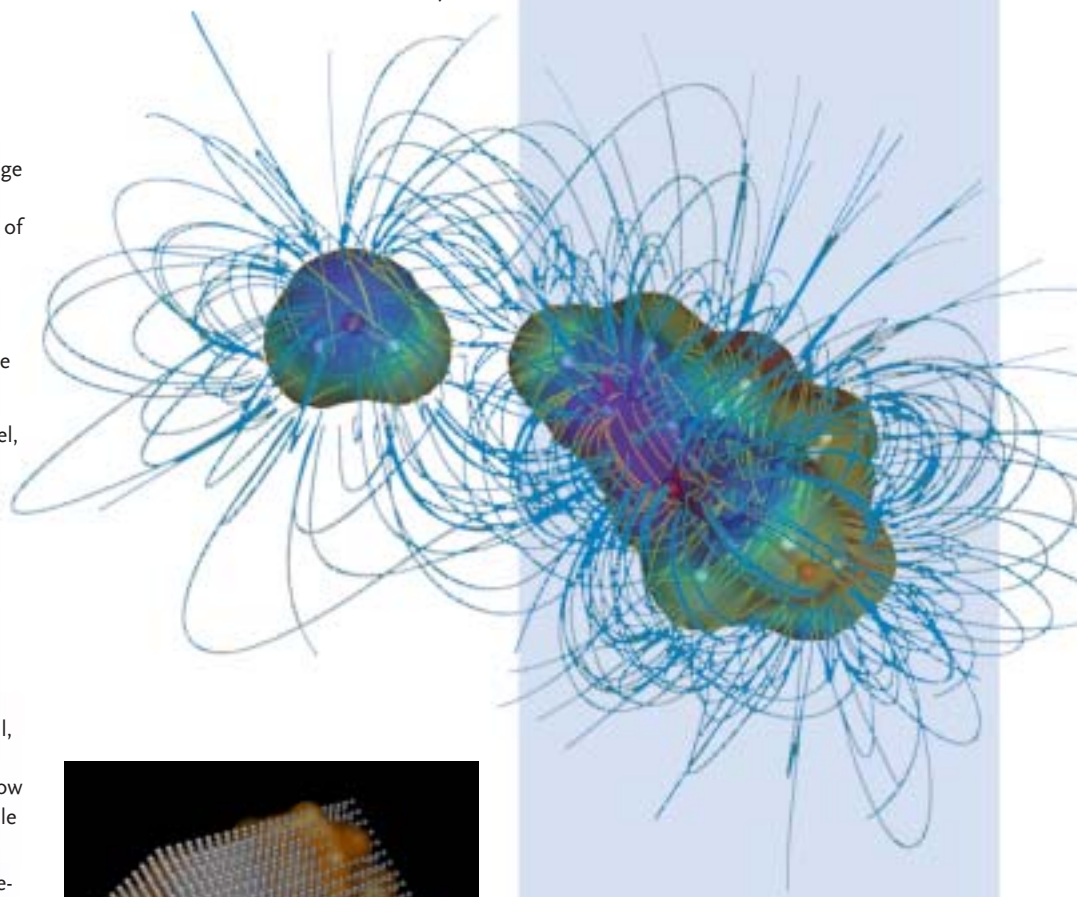


*Johann Gasteiger* is professor at the University of Erlangen-Nuremberg and a member of the editorial boards of different journals e.g. Journal of Chemical Information and Computer Sciences.

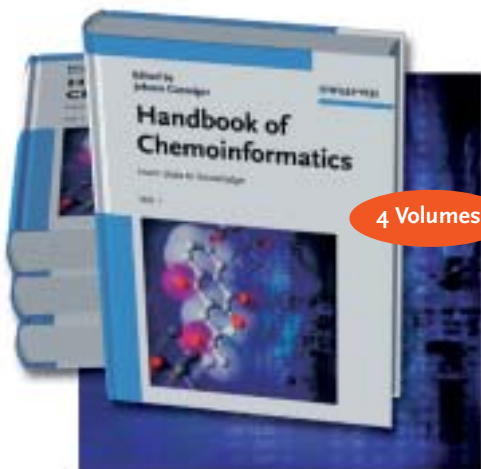
He is the recipient of the 1991 Gmelin-Beilstein Medal of the German Chemical Society for Achievements in Computer Chemistry, and the Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society (ACS) in 1997.



*Thomas Engel* joined the research group headed by Johann Gasteiger at the University of Erlangen-Nuremberg and is a specialist in chemoinformatics.



# The Reference Work



4 Volumes

Gasteiger, J. (ed.)  
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## Handbook of Chemoinformatics

From Data to Knowledge

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### Prepublication price

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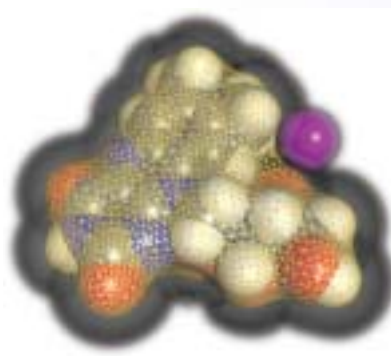
The applications cover a wide range, such as property prediction, spectra analysis and simulation, reaction prediction and synthesis design as well as drug design.

The accompanying textbook for students published separately is closely referenced to this set.

### From the contents

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- Introduction
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- Chemical Nomenclature and Structure Representation
- Processing Constitutional Information
- Representation of 3D Structures
- Molecular Shape Analysis
- Visualization in Molecular Science
- Representation of Chemical Reactions



### From Foreword of G.W.A. Milne

...Research in chemoinformatics enjoys powerful financial support, from an industry which sees its benefits very clearly and from governments which are determined to keep their countries' scientists on the cutting edge of development. Because of this, there is an explosion of results, leading to a steady flow of research publications and it is a significant challenge to develop a treatise that is much more than a snapshot of the current state of the science. Fortunately, the basics are not neglected here; in spite of all the progress, current research is not yet out of sight of the basics and we are therefore treated to a book which can stand alone for its valuable coverage of chemoinformatics.

#### VOLUME II

- Data Types
- Data Acquisition
- Standard Exchange Formats
- Databases of Chemical Structures
- Databases on Chemical Reactions
- Spectroscopic Databases
- Chemistry in the Internet
- Search Methods

#### VOLUME III

- Calculation of Physical and Chemical Data
- Molecular Mechanics
- Quantum Mechanics
- Descriptors for Chemical Compounds
- Methods for Data Analysis
- Expert Systems in Chemistry

#### VOLUME IV

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