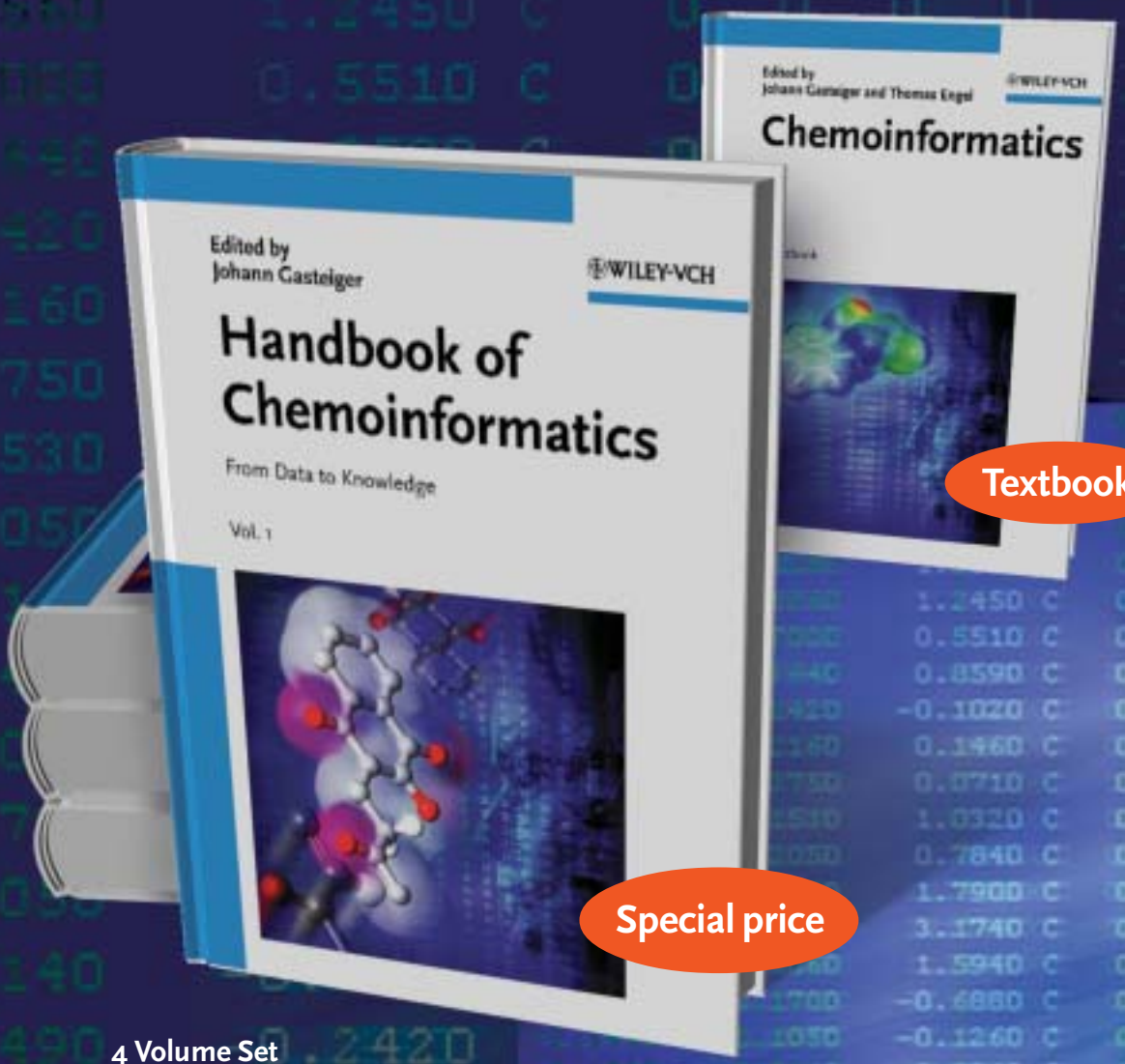
Setting the standard in

Chemoinformatics



Editors
Johann Gasteiger
& Thomas Engel

- Application-oriented
- Clearly structured
- Didactically brilliant

Textbook

Special price

4 Volume Set

Editor Johann Gasteiger

- Comprehensive
- High quality
- First in the field

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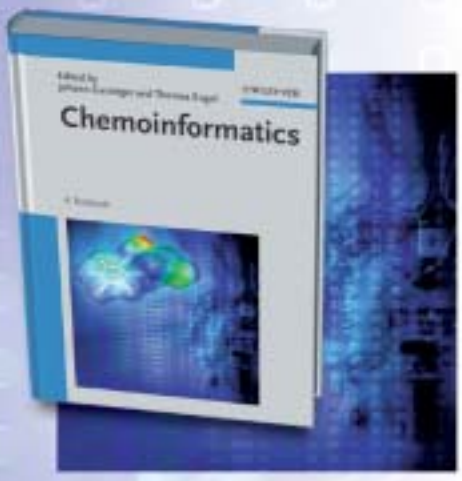
The Textbook



Gasteiger, J. / Engel, T. (eds.)
both from the University of
Erlangen-Nuremberg, Germany

Chemoinformatics

A Textbook

2003. Approx 450 pages. Softcover.
Approx € 69.00/£ 45.00/US$ 79.95
ISBN 3-527-30681-1

From the basics to applications - this is the first text to provide both students and newcomers to this exciting field with the knowledge and tools needed. Practical tutorials lead readers step-by-step through the entire range of chemoinformatic tools.

This first work to be devoted entirely to this increasingly important field, the "Textbook" provides both an in-depth and comprehensive overview of this exciting new area.

Edited by Johann Gasteiger and Thomas Engel, the book provides an introduction to the representation of molecular structures and reactions, data types and databases/data sources, search methods, methods for data analysis as well as such applications as structure elucidation, reaction simulation, synthesis planning and drug design. Clearly structured and didactically brilliant, the "Textbook" has an application-oriented approach and explains software tools in detail, such that students will not only learn the necessary theoretical background, but also how to use the different software packages available in the field.

For a more detailed presentation, users are referred to the "Handbook of Chemoinformatics", overleaf.

The Contents

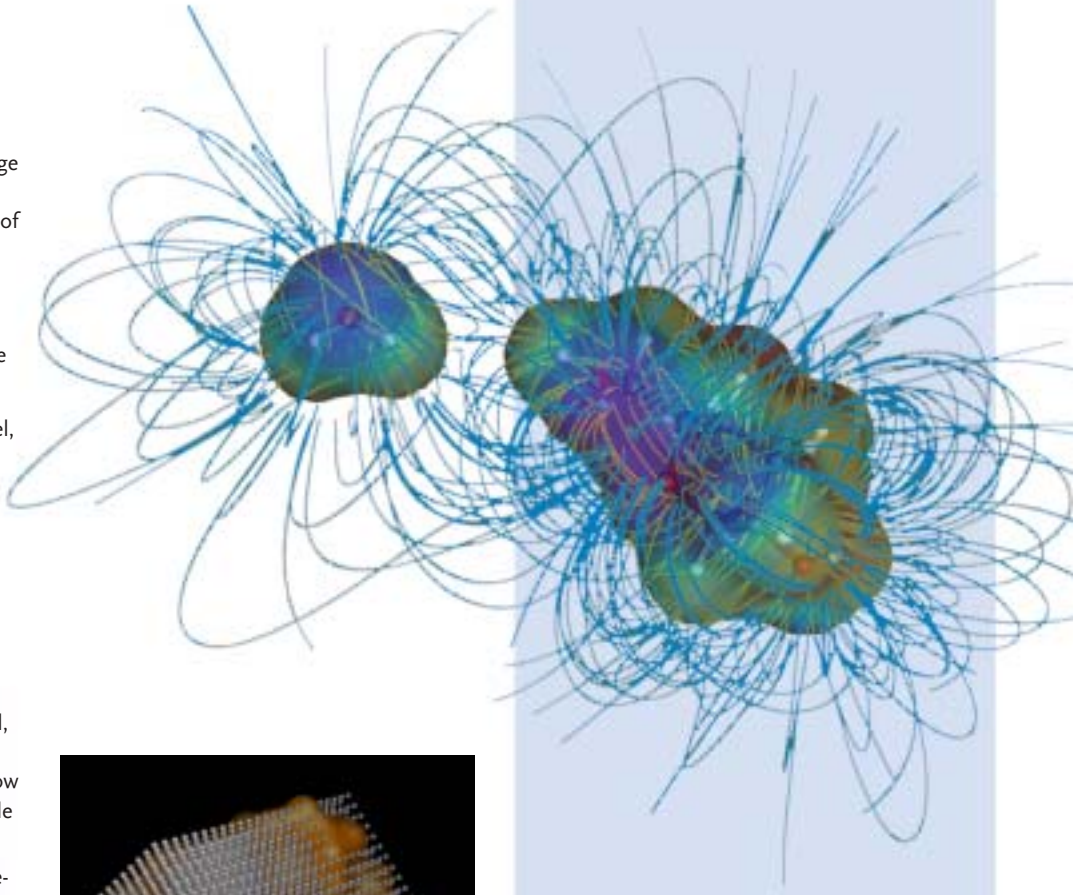
- Introduction
- Representation of Molecular Structures
- Representation of Chemical Reactions
- Search Methods
- The Data
- Databases/Datasources
- Calculation of Physicochemical Effects
- Calculation of Structure Descriptors
- Methods for Data Analysis
- Applications
- Future Directions

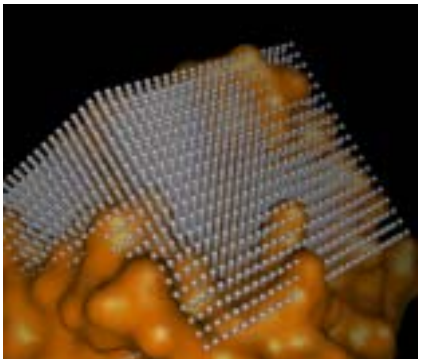
Readership

- Lecturers in chemistry
- Students in chemistry
- Chemists
- Computational chemists
- Medicinal chemists
- Biochemists
- Pharmaceutical industry
- Libraries

Fields

- Computational chemistry & molecular modeling
- Pharmaceutical & medicinal chemistry



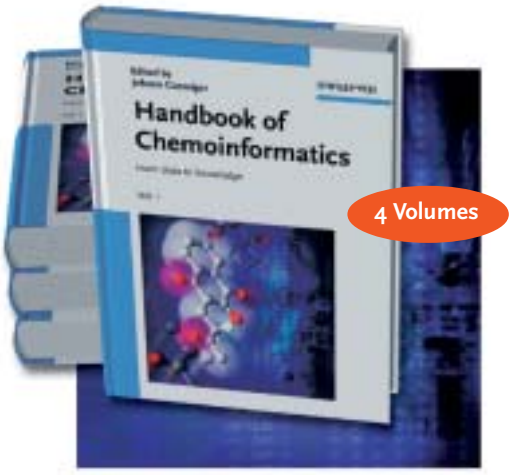


The Editors

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



Gasteiger, J. (ed.)
University of Erlangen-Nuremberg, Germany

Handbook of Chemoinformatics

From Data to Knowledge

2003. 1936 pages.
Hardcover. Four Volumes.
ISBN 3-527-30680-3

Prepublication price

Approx € 599.00/£390.00/US$ 675.00
valid until September 30th 2003, thereafter
approx € 699.00/£455.00/US$ 750.00

Everything chemists and other scientists need to know about this developing field – from data to knowledge. The "Handbook of Chemoinformatics" is the first reference work to be exclusively devoted to this exciting new area, and will set the standard as the premier information source for the next decade.

Edited by Johann Gasteiger, the four-volume handbook contains 73 in-depth contributions from 65 top authors from around the world, with the content organized into chapters dealing with the representation of molecular structures and reactions, data types and data bases/data sources, search methods, methods for data analysis as well as applications.

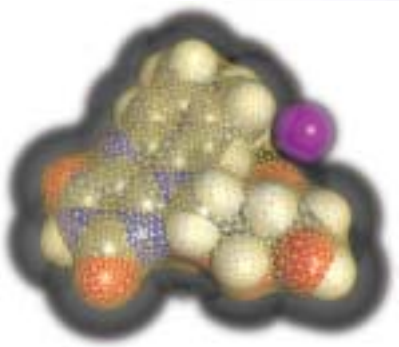
The applications cover a wide range, such as property prediction, spectra analysis and simulation, reaction prediction and synthesis design as well as drug design.

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

From the contents

VOLUME I

- Introduction
- History of Chemoinformatics
- Representation of Molecular Structures
- 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

- Prediction of Physical and Chemical Properties
- Structure-Spectra Correlations
- Chemical Reactions and Synthesis Design
- Drug Design
- Chemoinformatics/Bioinformatics
- Future Directions

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