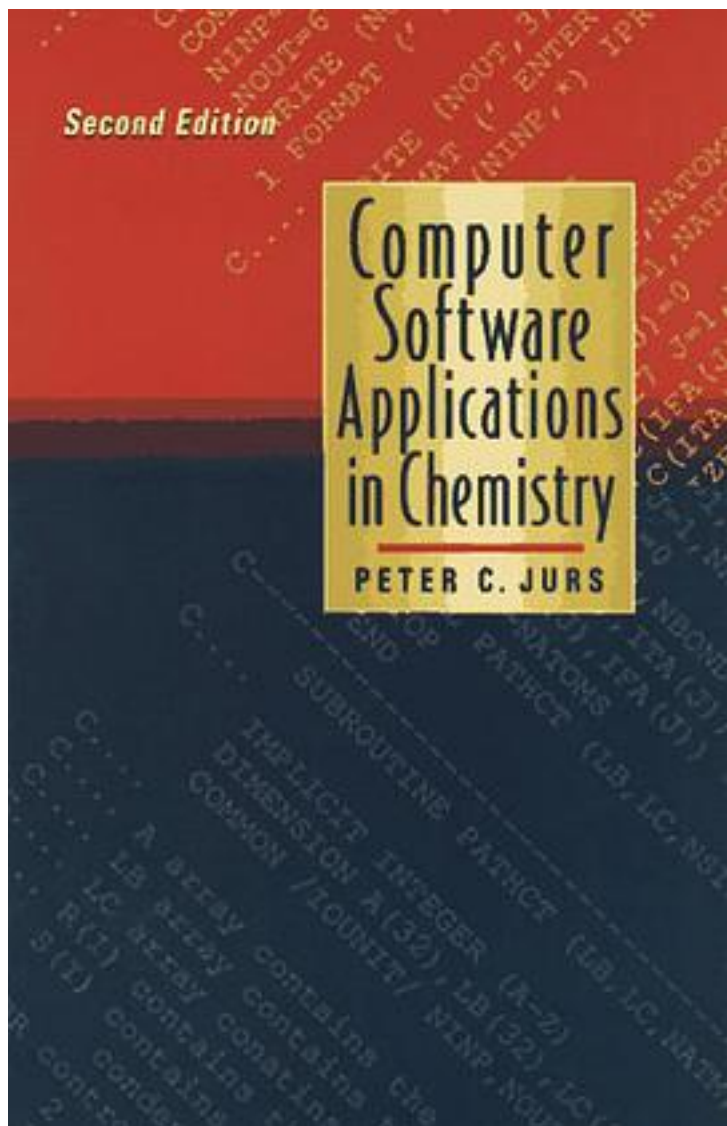# Computer Software Applications in Chemistry

[Computer Software Applications in Chemistry_下载链接1_](#)

著者:Peter C. Jurs

出版者:Wiley-Interscience

出版时间:1996-1-19

装帧:Hardcover

isbn:9780471105879

Intended specifically for practicing professionals and advanced students in chemistry and biochemistry, this invaluable book covers the full range of the computer applications in these fields, including numerical, nonnumerical, and graphics applications. New material includes multiple linear regression using MREG, principal-components analysis, Monte Carlo integration, parameterization of the force field, and molecular modeling software.

Major areas covered include:

* Error, Statistics, and the Floating-Point Number System

* Curve Fitting

* Multiple Linear Regression Analysis

* Numerical Integration

* Numerical Solution of Differential Equations

* Matrix Methods and Linear Equation Systems

* Random Numbers and Monte Carlo Simulation

* Simplex Optimization

* Chemical Structure Information Handling

* Mathematical Graph Theory

* Substructure Searching

* Molecular Mechanics and Molecular Dynamics

* Pattern Recognition

* Artificial Intelligence and Expert Systems

* Spectroscopic Library Searching and Structure Elucidation

* Graphical Display of Data and of Molecules

Whatever your area of research, this comprehensive, lucidly written book offers an indispensable resource of computer applications that will facilitate your work.

作者介绍:

目录:

标签

评论

[Computer Software Applications in Chemistry_下载链接1_](#)

书评

[Computer Software Applications in Chemistry_下载链接1_](#)

标签