The idea to write a textbook on chemometrics originated in my lecturing for undergraduate and graduate students. At the TU Bergakademie Freiberg, I have been giving lectures and computer exercises about chemometrics for almost 20 years, as well as lecturing as a visiting professor at other institutions, such as at the Vienna University of Technology on computer-based analytical chemistry (COBAC).

Over the years I’ve found that students work willingly and enthusiastically in chemometrics. The initial difficulties with the computer exercises are scarcely imaginable today, since many students arrive at the university more or less as computer freaks. Problems, however, are envisaged with respect to the appropriate evaluation of chemical measurements, because much statistical–mathematical knowledge is required. In most countries, unfortunately basic statistical and mathematical education of chemists is poor compared to that of, say, physicists.

Therefore, my textbook on chemometrics concerns the major topics in statistical–mathematical evaluation of chemical, especially analytical measurements. It is dedicated to the evaluation of experimental observations, but not to theoretical aspects of chemistry.

The book is subdivided into nine chapters. In the first chapter the subjects of chemometrics and their application areas are introduced. Chapter 2 provides the statistical fundamentals required to describe chemical data and to apply statistical tests. The methods of signal processing for filtering data and for characterizing data as time series are the subject of Chapter 3. In Chapter 4, the methods for effective experimentation based on experimental design and optimization are covered. The methods are outlined in such a way that they can be equally applied to optimize a chemical synthesis, an analytical procedure or a drug formulation. The methods of pattern recognition and the assignment of data sets in the sense of classification are presented in Chapter 5, which consists of sections on unsupervised and supervised learning. After introducing the methods of data preprocessing the typical chemometric methods for analysis of multidimensional data are outlined. Chapter 6 is dedicated to modeling of relationships ranging from straight-line regression to methods of multiple and nonlinear regression analysis. In Chapter 7, analytical databanks are discussed, i.e., the computer accessible representation of chemical structures and spectra including the use of LIMS systems. More recent developments in chemometrics are considered in Chapter 8. Apart from the fundamentals of artificial intelligence, the application of expert systems, of neural networks, of the theory of fuzzy sets and of genetic algorithms are discussed.
A very important topic for the actual application of statistical methods in the chemical laboratory is covered in Chapter 9: the most important methods for internal and external quality assurance, for validation, accreditation and for good laboratory practice.

In the Appendix the reader will find statistical tables, recommendations for software, and an introduction to linear algebra. The application of chemometric methods should be made easier by following the Learning objectives found in each chapter, by about 90 worked examples and by the Questions and Problems at the end of each chapter.

The textbook is not only written for chemometrics courses within the chemistry curriculum, but also for the individual study of chemists, pharmacists, mineralogists, geologists, biologists, and scientists of related disciplines. In this context, the book should be considered useful for colleagues from industry and it might be used, if, e.g., multivariate methods are needed to run a NIR spectrometer, to apply statistical tests in quality assurance or to investigate quantitative structure activity relationships.

As usual, the text would not have been written without the comments and suggestions of my colleagues in chemometrics. The first steps in using the computer application analytics I did together with Heinz Zwanziger many years ago, while later on I ran many courses on chemometrics together with Wolfhard Wegscheider; I would particularly like to acknowledge them both on this occasion.

In the second edition of the book I have increased the number of worked examples and extended the contents by more recent developments in chemometrics, such as wavelets, $N$-way analysis, support vector machines and simulated annealing or tabu search as global search strategies.

Finally, I like to thank the publisher Wiley-VCH in Weinheim for producing the book. I am especially grateful to Steffen Pauly who was again responsible for managing its edition.

January 2007

Matthias Otto