Preface

While modern techniques of nuclear magnetic resonance and mass spectrometry changed the ways of data acquisition and greatly extended the capabilities of these methods, the basic parameters, such as chemical shifts, coupling constants, and fragmentation pathways remain the same. This explains the ongoing success of the earlier editions of this book. However, since the amount of available data has considerably increased over the years, we decided to prepare an entirely new manuscript. It follows the same basic concepts, i.e., it provides a representative, albeit limited set of reference data for the interpretation of ^{13}C NMR, ^{1}H NMR, IR, mass, and UV/Vis spectra. On the other hand, the book has undergone a number of changes. The amount of reference data has been doubled at least (especially for MS and IR) and the order and selection of data for the various spectroscopic methods is now arranged strictly in the same way. In addition, the the enclosed compact disc contains programs for estimating NMR chemical shifts and generating isomers based on structural information.

Unfortunately, our teachers and colleagues, Prof. Wilhelm Simon and Prof. Thomas Clerc are no longer among us, and Prof. Joseph Seibl has retired years ago. Their contributions to developing the concept and the earlier editions of this work cannot be overemphasized. We also thank numerous colleagues who helped us in many different ways to complete the manuscript. We are particularly indebted to Dr. Dorothée Wegmann for her expertise with which she eliminated many errors and inconsistencies of the first versions. Special thanks are due to Dr. Rich Knochenmuss (ETH Zürich) for the MALDI mass spectra of matrix materials, Dr. Kikuko Hayamizu for her help with the Spectral Database System of the National Institute of Materials and Chemical Research, Tsukuba, Ibaraki (Japan), Prof. Bernhard Jaun and Dr. Martin Badertscher (ETH Zürich) for critically reading parts of the manuscript. Dr. Martin Badertscher is also thanked for the tutorial of the structure generator, Assemble 2.0, and Upstream Solutions (Hergiswil, Switzerland) for providing free versions of the computer programs on the enclosed compact disk.

In spite of great efforts and many checks to eliminate errors, it is likely that some errors or inconsistencies remain. We would like to encourage our readers to contact us with comments and suggestions or any kind of problems when using the book or the enclosed programs under one of the following addresses: Prof. Ernö Pretsch, Laboratory of Organic Chemistry, CH-8092 Zürich, Switzerland, e-mail: pretsch@org.chem.ethz.ch, or Prof. Philippe Bühlmann, Department of Chemistry, University of Minnesota, 207 Pleasant St., SE, Minneapolis, MN 55455, USA, e-mail: buhlmann@chem.umn.edu.

Zürich and Tokyo, August 2000