

1 Introduction

1.1 Scope and Organization

The present data collection is intended to serve as an aid in the interpretation of molecular spectra for the elucidation and confirmation of the structure of organic compounds. It consists of reference data, spectra, and empirical correlations from ^{13}C and ^1H nuclear magnetic resonance (NMR), infrared (IR), mass, and ultraviolet–visible (UV/vis) spectroscopy. It is to be viewed as a supplement to textbooks and specific reference works dealing with these spectroscopic techniques. The use of this book to interpret spectra only requires the knowledge of basic principles of the techniques, but its content is structured in a way that it will serve as a reference book also to specialists.

Chapters 2 and 3 contain Summary Tables and Combined Tables of the most relevant spectral characteristics of structural elements. While Chapter 2 is organized according to the different spectroscopic techniques, Chapter 3 provides for each class of structural elements spectroscopic information obtained with various techniques. These two chapters should assist users that are less familiar with spectra interpretation to identify the classes of structural elements present in samples of their interest. The following four chapters cover data from ^{13}C NMR, ^1H NMR, IR, and mass spectroscopy, and are ordered exactly in the same manner by compound types. These cover the various skeletons (alkyl, alkenyl, alkynyl, alicyclic, aromatic, and heteroaromatic), the most important substituents (halogen, single-bonded oxygen, nitrogen, sulfur, and carbonyl), and some specific compound classes (miscellaneous compounds and natural products). Finally, a spectra collection of common solvents, auxiliary compounds (such as matrix materials and references) and commonly found impurities is provided for each method. Not only the strictly analogous order of the data but also the optical marks on the edge of the pages help fast cross-referencing between the various spectroscopic techniques. Although currently, UV/vis spectroscopy is only marginally relevant to structure elucidation, its importance might increase by the advent of high throughput analyses. Also, the reference data presented in Chapter 8 are useful in connection with optical sensors and the widely applied UV/vis detectors in chromatography and electrophoresis.

Since a large part of the tabulated data either comes from our own measurements or is based on a large body of literature data, comprehensive references to published sources are generally not included. Whenever possible, the

data refers to conventional modes and conditions of measurement. For example, unless the solvent is indicated, the NMR chemical shifts were determined usually with deuteriochloroform or carbon tetrachloride as solvent. Likewise, the IR spectra were measured using solvents of low polarity, such as chloroform or carbon disulfide. Mass spectral data were recorded with electron impact ionization at 70 eV.

While retaining the basic structure of the previous editions, numerous new entries have been added. Altogether, the amount of data has been more than doubled. The section on mass spectrometry (MS) is entirely new and contains a unique collection of fragmentation rules for the various compound classes. As a new feature, prototype IR spectra for each class of compounds schematically show the analytically relevant absorption bands. The Combination Tables of the earlier editions have been extended and arranged in two chapters, the first organized according to band positions and the second according to compound classes.

The enclosed compact disc contains programs for estimating ^{13}C and ^1H chemical shifts of organic compounds containing up to 15 non-hydrogen atoms. Both programs are available for Windows and Macintosh systems and require a Java environment for the graphical structure input. Technical details about the requirements and installation procedures are given in the corresponding ReadMe files. Extensive help files are available as part of the programs. In addition, the structure generator Assemble 2.0 (also limited to 15 non-hydrogen atoms) is available for Windows systems. Based on the molecular formula and available structural information, it is capable of generating all possible structural isomers. An extensive hypertext based tutorial describes its main features. It is especially recommended as a quality control tool to check if alternative solutions that also agree with the experimental data have gone unnoticed.

1.2 Abbreviations and Symbols

al	aliphatic
alk	alkyl
alken	alkenyl
ar	aromatic
as	asymmetric
ax	axial
comb	combination frequency
d	doublet
δ	IR: deformation vibration
	NMR: chemical shift
DMSO	dimethyl sulfoxide
eq	equatorial
ϵ	molar absorptivity
Frag	fragment
γ	skeletal vibration
gem	geminal
hal	halogen
ip	in plane vibration
J	coupling constant
$M^{+\cdot}$	molecular radical ion
m/z	mass to charge ratio
v	frequency
oop	out of plane vibration
sh	shoulder
st	stretching vibration
sy	symmetric
TMS	tetramethylsilane
vic	vicinal