Pretsch · Clerc · Seibl · Simon

Tables of

Spectral Data for Structure Determination of Organic Compounds

^{13}C-NMR ^{1}H-NMR IR MS UV/VIS

Chemical Laboratory Practice

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Preface to the English Edition

Although numerical data are, in principle, universal, the compilations presented in this book are extensively annotated and interleaved with text. This translation of the second German edition has been prepared to facilitate the use of this work, with all its valuable detail, by the large community of English-speaking scientists. Translation has also provided an opportunity to correct and revise the text, and to update the nomenclature. Fortunately, spectroscopic data and their relationship with structure do not change much with time so one can predict that this book will, for a long period of time, continue to be very useful to organic chemists involved in the identification of organic compounds or the elucidation of their structure.

Klaus Biemann
Cambridge, MA, April 1983

Preface to the First German Edition

Making use of the information provided by various spectroscopic techniques has become a matter of routine for the analytically oriented organic chemist. Those who have graduated recently received extensive training in these techniques as part of the curriculum while their older colleagues learned to use these methods by necessity. One can, therefore, assume that chemists are well versed in the proper choice of the methods suitable for the solution of a particular problem and to translate the experimental data into structural information.

Those who are not specialists in any of these techniques and therefore not in continuous contact with the corresponding data may wish to have a compact summary of reference data in a form that can be grasped easily. Even experts appreciate the opportunity to look up

in a summary information about compound types with which they are not familiar. The tables compiled in this book are meant to fill this gap. They were compiled for courses and exercises which the authors offered over a ten year period to students at the Federal Institute of Technology (ETH), Zurich, and are thus well suited as a basis for similar courses elsewhere.

Considering such a broad effort there will undoubtedly be some omissions and errors in our presentations. We would be grateful to users of this book for suggestions and criticisms which would help us to keep it up to date. A postcard included in the book may make it easier for the reader to make such comments. We would also be grateful to receive reprints of papers containing information and data which could be incorporated in later editions and thus improve their usefulness.

A book such as this could not be assembled without the help of enthusiastic and knowledgeable collaborators who contributed a good deal to the work. Our special thanks go to Miss I. Port, Dr. D. Wegmann as well as Mr. P. Oggenfuss and Dr. R. Schwarzenbach.

Preface to the Second German Edition

This second edition provided an opportunity to include many additions and correct some errors. Amongst other improvements tables and figures concerning opaque regions and error-signals in the infrared were added. We also appreciate correspondence which led to a number of corrections.

Our special thanks go to Dr. D. Wegmann and Mr. P. Oggenfuss for their very careful cooperation. It is due to their efforts that this new edition was produced in a timely fashion.

Introduction

The following collection of data is intended to serve as an aid in the interpretation of ^{13}C- and ^{1}H-nuclear magnetic resonance, infrared, mass and electron excitation spectra. It is to be viewed as an addition to texts and reference works dealing with these spectroscopic techniques. It is designed for those who are routinely faced with the task to interprete this type of spectral information. The use of this book for the interpretation of spectra requires only the knowledge of basic principles of these techniques, but its content is structured in a way that it will also serve as a reference work for the specialist.

To aid rapid access to relevant data the following codes are listed at the top of the appropriate pages:

KOMB: Summary of characteristic spectroscopic data arranged by structural elements.
(pages B5 through B265)

^{13}C-NMR: ^{13}C-nuclear magnetic resonance spectral data ordered by compound types.
(pages C5 through C265)

^{1}H-NMR: Proton magnetic resonance spectral data.
(pages H5 through H370)

IR: Infrared absorption frequencies ordered by functional groups or compound types.
(pages I5 through I280)

MS: Tables and suggestions for the interpretation of mass spectra.
(pages M5 through M170)

UV/VIS: Tables, suggestions and reference spectra for rationalization of electron excitation spectra.
(pages U5 through U155)

The tables are arranged as much as possible in an analogous manner for all methods, but the details of the presentation are dictated by the characteristics of the individual technique.

The pages are numbered in increments of five which should facilitate later additions.

The summaries presented on pages B5 through B70 facilitate the recognition of first-cut conclusions concerning the structure by those users less familiar with such interpretations, particularly in those cases where no ancillary information is available. The tables presented on pages B75 through B245 make it possible to check in a second step the suspected structural elements for the most important compound types. The remaining tables make it possible to predict the spectroscopic characteristics of a proposed compound. They also serve as a reference compilation for the correlation of the structure of organic compounds with the corresponding spectral data.

Because a large part of the tabulated data is from our own measurements and the rest is based on a large body of literature data a comprehensive reference to published sources is not included. Whenever possible the data refer to conventional modes and conditions of measurement. For example, the chemical shifts for NMR spectra were determined generally in deuterochloroform or carbon tetrachloride. The wave numbers (IR) refer to solvents of low polarity, such as chloroform or carbon disulfide. Mass spectral data were recorded at an electron energy of 70 eV. Most of the data were taken from the following sources:

Batterham, T.J.: NMR spectra of simple heterocycles. New York - London - Sydney - Toronto: Wiley-Interscience 1973.

Bhacca, N.S., Hollis, D.P., Johnson, L.F., Pier, E.A., Shoolery, J.N.: NMR spectra catalog. Varian Associates 1962 and 1963.

Bremser, W., Ernst, L., Franke, B.: Carbon-13 NMR spectral data. 2nd ed. Weinheim: Verlag Chemie 1979.

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Yukawa, Y.: Handbook of organic structural analysis. New York - Amsterdam: W.A. Benjamin 1965

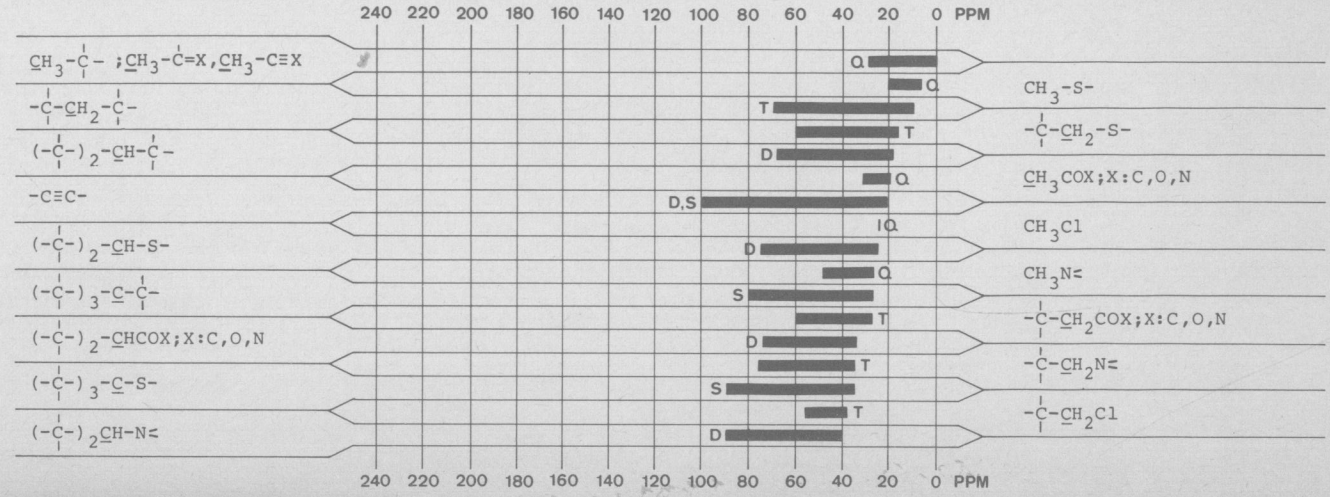
Abbreviations and Symbols

al	aliphatic
ar	aromatic
as	asymmetric
ax	axial
comb	combination frequency
δ	IR: deformation frequency NMR: chemical shift
eq	equatorial
γ	skeletal vibration
gem	geminal
hal	halogen
ip	"in plane" vibration
oop	"out of plane" vibration
st	stretching vibration
sy	symmetric

Table of Contents

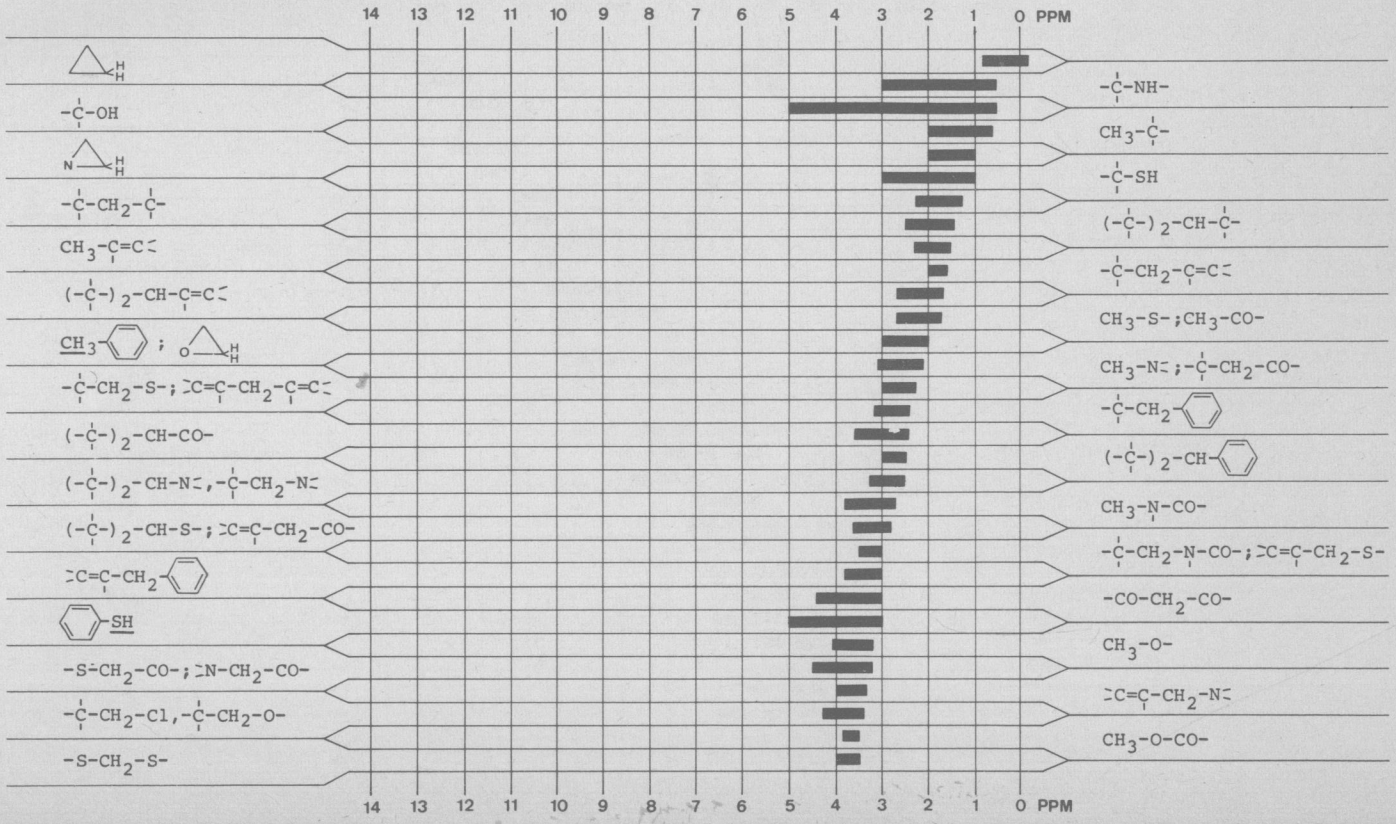
Summary of the Regions of the Chemical Shifts for Carbon in Various Bonding Environments
(δ in ppm relative to TMS)

The multiplicity of "off-resonance" uncoupled first order spectra is indicated by the following abbreviations: S = singlet, D = doublet, T = triplet, Q = quadruplet

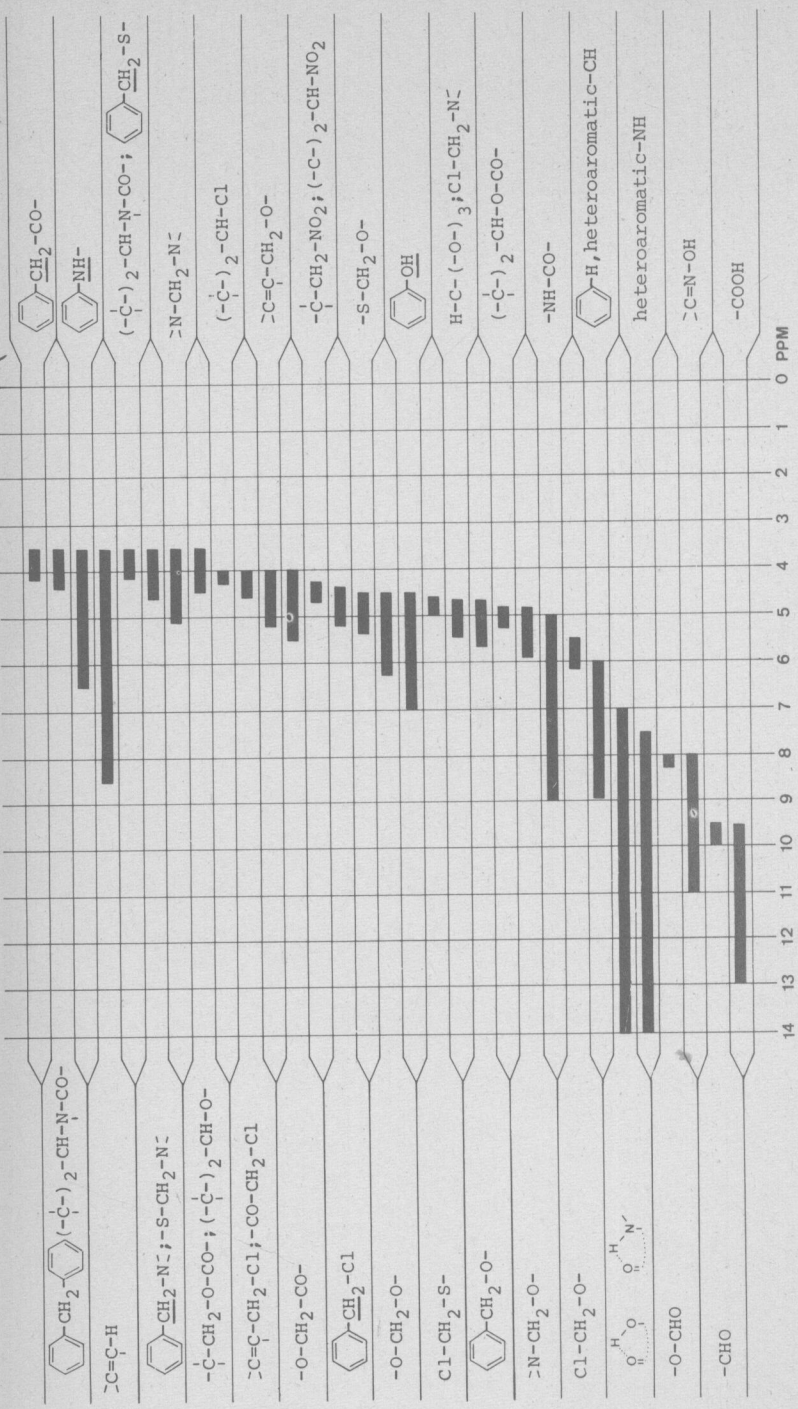


^{13}C-NMR, SUMMARY

Summary of the Regions of the ^{1}H Chemical Shifts of Protons in Various Bonding Environments (δ in ppm relative to TMS)



^{1}H-NMR, SUMMARY



^{1}H-NMR, SUMMARY

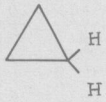
Summary of Ranges of Coupling Constants Between Differently Bound Protons (|J| in Hz)

X and Y represent different substituents.

Geminal coupling:

10 - 14

0 - 20



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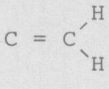
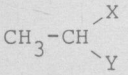


0 - 4

Vicinal coupling:



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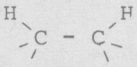

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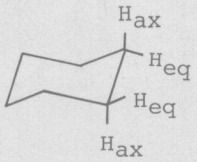

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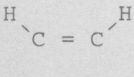
ax,eq: 2 - 4
eq,eq: 2 - 4



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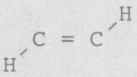

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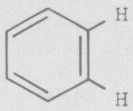

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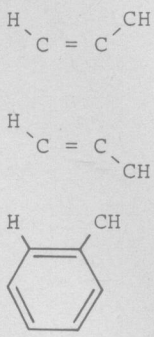
"Long-range" coupling:



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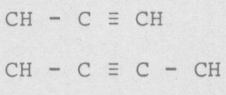

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