CARBON-13
NMR
SPECTROSCOPY

Hans-Otto Kalinowski
Stefan Berger
Siegmar Braun

Carbon-13 NMR Spectroscopy

HANS-OTTO KALINOWSKI
Institute for Organic Chemistry
Justus Liebig University
Giessen
Federal Republic of Germany

STEFAN BERGER
Department of Chemistry
University of Marburg
Federal Republic of Germany

SIEGMAR BRAUN
Institute for Organic Chemistry and Biochemistry
Technical University of Darmstadt
Federal Republic of Germany

Translated by Jack K. Becconsall

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Preface

Twenty-seven years after the recording of the first ^{13}C NMR spectrum, and more than thirteen years after the introduction of the first commercial ^{13}C spectrometer, this branch of spectroscopy has not only become an established and well documented technique, but is also beginning to yield even more detailed information on increasingly complex organic and biological systems, through the possibilities opened up by pulse techniques.

The authors' intention is to describe the technique at this stage of development, with regard to both the methods and their application to chemical problems. All three authors are organic chemists and are active in the practice and application of ^{13}C NMR spectroscopy, being in charge of NMR spectroscopy laboratories in various academic institutes. The present book, based on material prepared for lectures, courses and seminars, is suitable mainly for organic chemists, especially for those engaged in research, and also diploma and doctoral postgraduate students.

Consequently, prominence is given to the treatment of the structural dependence of NMR parameters, namely the ^{13}C chemical shift, ^{13}C–X spin–spin couplings and to a lesser extent the relaxation time T_1. These chapters are preceded by an introduction to the physical basis of nuclear magnetic resonance experiments, and a detailed description of those measurement techniques which are peculiar to the pulsed Fourier transform (PFT) technique generally used for heteronuclides such as ^{13}C. The classical procedure of continuous irradiation (c.w. method) is not treated at all. A fair amount of detail in this section seemed to us entirely appropriate, even for the practical user, because in the PFT method the path between the information contained in a nuclear spin system and the resulting spectrum which mirrors this information is especially long and can be full of pitfalls. An insight into this connection should enable the user to look more critically at most ^{13}C NMR spectra measured in the course of routine service work, and to extend the range of experimental methods that can be used in solving his problem. Further, a sound base of knowledge should make it possible to gain a better insight into the constantly growing number of new types of pulse experiments.

The authors have been especially concerned to give the reader as direct an access to original publications as is possible. To each chapter we have added an extensive bibliography, which also provides information on the origins of the data. In our efforts to include references as recent as possible, while embracing the earlier literature and avoiding too large a number, it has naturally not always been possible to take account of the usual considerations on priority.

We have used the SI system throughout, and have accordingly employed the symbol B_0. We have, however, followed the common (incorrect) usage in referring to the latter as the magnetic field rather than the magnetic induction.

[*Translator's note*: The name 'magnetic flux density' for B_0 is unambiguous, and is gaining wider acceptance. I have, however, followed the authors throughout this book by using 'magnetic field'.]

In the treatment of ^{13}C chemical shifts, we did not set out to give general rules and then merely to exemplify these by reference to a few particular systems with a limited range of substituents. Instead, we have systematically treated each class of compounds in turn, as in a textbook of organic chemistry, and in addition to their specific characteristics and any incremental relationship that has been developed, the data for many individual compounds are listed. The need to limit the size of the compilation has been achieved by concentrating mainly on the ^{13}C chemical shifts of the simpler compounds, while more complex structures such as natural products, and structures such as transition metal complexes which are on the fringes of organic chemistry, have been less thoroughly treated. In analysing substituent effects on ^{13}C chemical shifts, incremental relationships based on α-, β-, γ-, ..., effects have been given preference over linear equations, as the former are better in giving a consistent picture related to the chemist's view of structure. Besides expressions such as 'a shift to higher (or lower) frequency,' we shall also employ the terms 'downfield shift' or 'upfield shift,' which are deeply rooted in laboratory usage, even though PFT measurements are made at a constant magnetic field strength; the corresponding chemical shift changes $\Delta\delta$ have positive and negative signs, respectively.

Likewise, the structural dependence, and especially the stereochemical aspects, of the couplings between ^{13}C nuclei and other nuclei with spin $I = \frac{1}{2}$, have been treated more thoroughly than usual. The ^{13}C–X spin–spin interactions $J(^{13}C,X)$ have in recent years assumed great importance as structural parameters, where the coupling partner can be ^{1}H, ^{13}C itself or one of the commonly occurring spin-½ nuclides, ^{19}F or ^{31}P. This development is due in no small part to the increased sensitivity and dispersion of the modern high-field spectrometer, as well as to new operational techniques. The main emphasis has been put on the couplings of ^{13}C with the four above-named elements, owing to their importance in organic chemistry, with the addition of ^{15}N, even though ^{15}N enrichment for observing ^{13}C–^{15}N couplings is not yet common. Fewer details are given on couplings with other Main Group elements that occur in typical organometallic compounds, whilst we have touched only briefly on the transition metal elements as coupling partners of ^{13}C.

Since the ^{13}C nuclide is central to this book, we have departed from the generally recommended convention by always naming ^{13}C first in describing a coupling, even when the coupling partner is a heavier element. Thus, for example, we write not only $J(^{13}C,^{7}Li)$ and $J(^{13}C,^{11}B)$, but also $J(^{13}C,^{15}N)$ (see above), $J(^{13}C,^{31}P)$, and so on. Also, in couplings with deuterium, we have used the symbol D rather than ^{2}H for easier readability and a clearer distinction from ^{1}H.

Further, in contrast to the chapter on chemical shifts, we have treated spin–spin couplings not under compound classes, but under types of couplings $^{n}J(^{13}C,X)$, with $n = 1,2,3,\ldots$ Following to some extent the practice for H–H couplings, we refer to these respectively as one-bond, geminal, vicinal and long-range ($n \geqslant 4$) couplings. Although their signs are not in general directly apparent from the spectra, we have paid regard to them wherever possible, since only in this way can they be compared and used, for example, to recognize structural similarities.

So as to consolidate and broaden the material presented, exercises have been appended to the individual sections. The solutions are either given in Appendix A, or can be looked up in the original papers with the help of the references given.

We invite comments and suggested improvements to the work, which are always welcomed.

Finally, we thank the publishers for their excellent cooperation and understanding with regard to the authors' desire to incorporate as much detail and visual clarity as possible into the structural formulae of the many compounds included.

Our special thanks go to Prof. Dr. H. Günther of Siegen, Dr. F. K. Bär of Marburg and Dr. K. Wilhelm of Münster for their critical reviews of parts of the manuscript.

January 1984

H.-O. Kalinowski
Giessen

S. Berger
Marburg

S. Braun
Darmstadt

Preface to the English Edition

The authors are very pleased that, following the publication of the German version, an English translation is now appearing which will allow the book to reach a wider readership. We have taken this opportunity to look critically at the material, and it has been possible to take up some suggestions which we received from readers of the German edition. Thus, in view of the continuing rapid developments in modern pulse techniques, Chapter 2 has been brought up to date, and in Chapter 3 the most recent literature has been included in the form of additional references in the bibliographies attached to the various sections. The section on ^{13}C–^{13}C couplings in Chapter 4 has been rewritten, and in Chapters 5–8 the latest published work has been incorporated. Lastly, the opportunity has been taken to eliminate a number of misprints and errors.

We wish especially to thank all those who have contributed to the improvement of the book in its English edition. We also welcome any further suggestions for improvements!

Our thanks are also due to the publishers, who have been willing to accommodate our wishes for improvements, and to the translator, who also provided suggestions and completed the work in the shortest possible time.

May 1986

H.-O. Kalinowski Giessen	*S. Berger* Marburg	*S. Braun* Darmstadt

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Chapter 1

Foundations of magnetic resonance

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2. **Quantization of angular momentum**
3. **Relationship between angular momentum and magnetic moment**
4. **Energy of a nuclear spin in a magnetic field**
5. **The Larmor frequency**
6. **The nuclear resonance experiment**
7. **Energy level populations and nuclear spin relaxation**
8. **The Bloch equations**

1. Historical development

The first experimental demonstration of the directional quantization of an electron spin was achieved by Stern and Gerlach[1] in 1924, using a beam of silver atoms. Fifteen years later, Rabi *et al.*,[2] using a beam of lithium chloride molecules, carried out the first magnetic resonance experiment, which gave evidence for the existence of the nuclear spin. Eventually, in 1945, Purcell and Bloch and their collaborators[3,4] discovered the nuclear resonance effect in condensed matter (1952 Nobel Prize).

These physics experiments first started to become of great interest for chemistry with the discovery of the chemical shift,[5] for this made it possible to use the NMR technique as a practical spectroscopic method for studying chemical compounds.

The introduction of the first commercial NMR spectrometers since 1953 was followed by a remarkable growth of this new technique, primarily in proton resonance.

A second, equally important, step forward in the development of the NMR method began at the start of the 1970s. Although Lauterbur[6] had obtained the first ^{13}C NMR spectrum as early as 1957, recording such spectra was very laborious, and confined to only a few laboratories. The reasons for this were the ^{13}C nuclide's low natural abundance of 1.1%, and its small gyromagnetic ratio γ, less than that of the proton by a factor of 4. Since the gyromagnetic ratio appears as γ^3 in the expression for the relative sensitivity for a given nuclide, the ^{13}C resonance is about a factor of 6000 weaker than that of the proton.[7]

Some improvements were achieved by the introduction of proton decoupling and data accumulation, made possible by the development of field-frequency stabilization using an NMR signal (NMR lock).

The decisive breakthrough for ^{13}C resonance did not arrive until Ernst and Anderson,[9] following the preliminary work by Lowe and Norberg,[8] introduced the pulsed Fourier transform (PFT) technique into NMR spectroscopy.

Meanwhile, it had become standard practice in the chemical literature to verify new structural findings for carbon-containing compounds by including ^{13}C NMR data.

During the early 1980s, most NMR laboratories were able to replace their first- and second-generation FT NMR spectrometers by modern spectrometers, which typically employ a superconducting magnet and have a dedicated computer integrated into the system. Along with this development, the exploration of new pulse techniques has resulted in advances at a bewildering rate.

In view of this state of development, our description of the foundations of magnetic resonance in Chapter 1 and of experimental methods in Chapter 2 will be devoted exclusively to pulse techniques.

2. Quantization of angular momentum

As a consequence of the postulates of quantum mechanics, the angular momentum of any isolated particle, such as an atomic nucleus, cannot take any random value. Its magnitude is specified by a nuclear spin quantum number I according to

$$|\boldsymbol{p}| = \hbar\sqrt{I(I+1)}$$

$$\left[\hbar = \frac{h}{2\pi}\right] \qquad (1.1)$$

Since the angular momentum $\boldsymbol{p}$ is represented by a vector quantity, to specify it fully we must give the direction as well as the magnitude. However, relative to some chosen direction, which we will arbitrarily take as the z-axis of a Cartesian coordinate system, the vector cannot assume any random orientation. Its position is specified by introducing a magnetic quantum number m_I, such that the vector's projection p_z must satisfy the equation

$$p_z = \hbar m_I \qquad (1.2)$$

In Eq. 1.2, m_I can take any of the values from $-I$ in steps of 1 to $+I$:

$$m_I = I, I-1, I-2, \ldots, -I \qquad (1.3)$$

Hence there are $2I + 1$ allowed values for the projection of the angular momentum on to the chosen direction. The situation for a particle with spin quantum number $I = ½$, as is the case for the ^{13}C nucleus, is illustrated in Fig. 1.1.

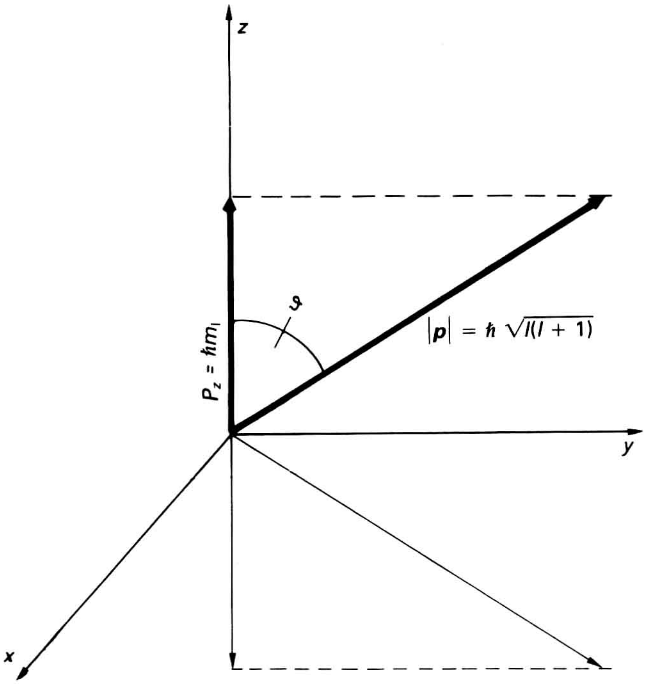

Fig. 1.1 Directional quantization of angular momentum

It follows from this representation that the angle θ between the vector $\boldsymbol{p}$ and its projection on the z-axis is given by

$$\cos\theta = \frac{m_I}{\sqrt{I(I+1)}} \tag{1.4}$$

3. Relationship between angular momentum and magnetic moment

It turns out that nuclides with even mass number and even atomic number, e.g. ^{12}C or ^{16}O (even–even nuclides), all have zero nuclear angular momentum, i.e. zero spin, whereas nuclides with odd mass or atomic number, e.g. ^{1}H, ^{13}C, ^{17}O (odd–even, even–odd or odd–odd nuclides), all exhibit a nuclear spin.

According to the laws of classical physics, motion of electric charge causes a magnetic field. If the electric current flows around a closed loop, it has associated with it a magnetic dipole moment.

These considerations also apply in principle to atomic nuclei, and consequently nuclei with a nuclear spin also possess a magnetic moment $\boldsymbol{\mu}$, which according to Eq. 1.5 is proportional to the angular momentum.

$$\boldsymbol{\mu} = \gamma \boldsymbol{p} \tag{1.5}$$

The quantity γ is called the gyromagnetic ratio, and can be measured directly from the nuclear resonance experiment. Table 1.1 lists γ values for a few nuclides.

Table 1.1 Values of γ and other properties for various nuclides

Isotope	Spin	Natural abundance (%)	γ ($\times 10^{7}$ rad $T^{-1}s^{-1}$)	NMR frequency at 2.3487 T (MHz)	Quadrupole moment, Q ($\times 10^{-28}$ m^{2})
^{1}H	$\frac{1}{2}$	99.98	26.751	100.0	
^{2}H	1	0.015	4.1064	15.351	2.73×10^{-3}
^{6}Li	1	7.42	3.9366	14.716	6.9×10^{-4}
^{7}Li	$\frac{3}{2}$	92.58	10.396	38.862	-3×10^{-2}
^{10}B	3	19.58	2.8748	10.747	7.4×10^{-2}
^{11}B	$\frac{3}{2}$	80.42	8.583	32.084	3.55×10^{-2}
^{13}C	$\frac{1}{2}$	1.108	6.7263	25.144	
^{14}N	1	99.63	1.9324	7.224	1.6×10^{-2}
^{15}N	$\frac{1}{2}$	0.37	$-$ 2.7107	10.133	
^{17}O	$\frac{5}{2}$	0.037	$-$ 3.6266	13.557	-2.6×10^{-2}
^{19}F	$\frac{1}{2}$	100	25.1666	94.077	
^{23}Na	$\frac{3}{2}$	100	7.076	26.451	0.14
^{29}Si	$\frac{1}{2}$	4.7	$-$ 5.314	19.865	
^{31}P	$\frac{1}{2}$	100	10.829	40.48	
^{35}Cl	$\frac{3}{2}$	75.53	2.6212	9.798	-7.89×10^{-2}
^{37}Cl	$\frac{3}{2}$	24.47	2.182	8.156	-6.21×10^{-2}
^{57}Fe	$\frac{1}{2}$	2.19	0.8644	3.231	
^{77}Se	$\frac{1}{2}$	7.58	5.101	19.068	
^{79}Br	$\frac{3}{2}$	50.54	6.7021	25.054	0.33
^{81}Br	$\frac{3}{2}$	49.46	7.2245	27.006	0.28
^{89}Y	$\frac{1}{2}$	100	$-$ 1.3106	4.899	
^{103}Rh	$\frac{1}{2}$	100	$-$ 0.842	3.147	
^{107}Ag	$\frac{1}{2}$	51.82	$-$ 1.0825	4.046	
^{109}Ag	$\frac{1}{2}$	48.18	$-$ 1.2445	4.652	
^{111}Cd	$\frac{1}{2}$	12.75	$-$ 5.6727	21.205	
^{113}Cd	$\frac{1}{2}$	12.26	$-$ 5.934	22.182	
^{117}Sn	$\frac{1}{2}$	7.61	$-$ 9.5301	35.625	
^{119}Sn	$\frac{1}{2}$	8.58	$-$ 9.9708	37.27	
^{127}I	$\frac{5}{2}$	100	5.351	20.007	-0.69
^{169}Tm	$\frac{1}{2}$	100	$-$ 2.213	8.272	
^{171}Yb	$\frac{1}{2}$	14.31	4.712	17.614	
^{183}W	$\frac{1}{2}$	14.4	1.1131	4.161	
^{187}Os	$\frac{1}{2}$	1.64	0.616	2.303	
^{195}Pt	$\frac{1}{2}$	33.8	5.75	21.494	
^{199}Hg	$\frac{1}{2}$	16.84	4.769	17.827	
^{205}Tl	$\frac{1}{2}$	70.5	15.438	57.71	
^{207}Pb	$\frac{1}{2}$	22.6	5.5968	20.92	