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Chemical Shifts and Coupling Constants for Hydrogen-1 NMR

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Hydrogen-1 NMR data

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Preface

Nuclear Magnetic Resonance (NMR) is based on the fact that certain nuclei exhibit a magnetic moment, orient by a magnetic field, and absorb characteristic frequencies in the radiofrequency part of the spectrum. The spectral lines of the nuclei are highly influenced by the chemical environment i. e. the structure and interaction of the molecules. Magnetic properties of nuclei have been known since 1924 and the first Nuclear Magnetic Resonance experiment has been made in 1945.

NMR is now the leading technique and a powerful tool for the investigation of the structure and interaction of molecules. The present Landolt-Börnstein volume III/35 "Nuclear Magnetic Resonance (NMR) Data" is therefore of major interest to all scientists and engineers who intend to use NMR to study the structure and the binding of molecules.

In contrast to the 6th Edition of Landolt-Börnstein it is nowadays impossible to include the complete data in the printed version. The aim of the New Series Edition of Landolt-Börnstein is therefore to store all data and references in electronic files and selected data and references in the printed version. The editors have decided to include the complete chemical shifts in the printed version with respect to this volume. The electronic version on the CD-ROM contains both the complete chemical shifts and the coupling constants.

Volume III/35 "NMR-Data" is divided into several subvolumes and parts. Subvolume III/35A contains the nuclei ^{11}B and ^{31}P , subvolume III/35B contains the nuclei ^{19}F and ^{15}N , subvolume III/35C contains the nucleus ^1H , and subvolume III/35D contains the nucleus ^{13}C . The nucleus ^{17}O and other nuclei will be presented later. Subvolume III/35C is divided into four parts. The present III/35C Part 1 includes aliphatic and aromatic hydrocarbons, steroids, and carbohydrates, the second part includes heterocycles, the third part includes natural compounds and the fourth part includes inorganic and organometallic compounds.

The chemical shifts δ (in ppm) and the coupling constants J (in Hz) are given along with the complete references. The data are arranged according to the compounds. The arrangement of the compounds is based on their gross formulae and are arranged according to the widely used Hill system. Additionally the complete structural formulae are given for all compounds.

The complete data including the structural formulae are available on the provided CD-ROM as PDF-files together with the program Adobe Acrobat Reader 3.0. You have to install only this program to jump directly into the data files and search for substances, references, chemical shifts, coupling constants and so on by the fulltext search engine. Additionally it would be possible to get the computerized data from the electronic version for numerical calculations and graphical presentations.

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Survey of Volume III/35

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Chemical Shifts and Coupling Constants
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Subvolume D

1 Introduction

The phenomenon of nuclear magnetic resonance (NMR) is based on magnetic properties of nuclei and therefore they are included here.

1.1 Magnetic properties of nuclei

All nuclei carry a charge and in some nuclei this charge spins on the nuclear axis generating a magnetic field along the axis. These nuclei behave as tiny bar magnets. The magnetic properties of a nucleus can be specified in terms of spin number I ($I = 0, 1/2, 1, 1\frac{1}{2}, 2, 2\frac{1}{2}, \dots$) and magnetic moment μ of the nucleus. The magnetic moment of the nucleus is proportional to the spin angular momentum and is expressed by Eq. (1) :

$$\mu \propto [I(I+1)]^{1/2} h/2\pi , \quad (1)$$

$$\mu = \gamma [I(I+1)]^{1/2} h/2\pi , \quad (2)$$

where γ is a proportionality constant known as gyromagnetic or magnetogyric ratio (differing for each nucleus and essentially measures the strength of nuclear magnets). $[I(I+1)]^{1/2} h/2\pi$ is the spin angular momentum in terms of spin number I , h is Planck's constant ($6.626 \cdot 10^{-34}$ J/s).

However, the measurable component of the angular momentum is $I h/(2\pi)$ and Eq. (2) can be reduced to Eq. (2a) :

$$\mu \approx \frac{\gamma h I}{2\pi} . \quad (2a)$$

The magnetic moment μ can be also expressed in terms of the Bohr magneton (or nuclear magneton) by Eq. (3) :

$$\mu = g_n B_n [I + (I+1)]^{1/2} h/(2\pi) , \quad (3)$$

where g_n is known as nuclear g -factor (which is being determined experimentally). B_n is the nuclear magneton defined as $\frac{e h}{4\pi m}$ (e = electronic charge, m = mass of proton) = $5.05 \cdot 10^{-24}$ erg/G.

Each proton and neutron has its own spin and spin number. I is the resultant of these two spins. If the sum of protons and neutrons (i.e. mass number) is odd, I is half-integer ($I = 1/2, 3/2, 5/2, \dots$), if both protons and neutrons are even-numbered, I is zero ($I = 0$ denotes no spin) and if the sum is even, I is integer ($I = 1, 2, 3, 4, \dots$). The magnetic properties of some NMR nuclei are summarized in Table 1. Nuclei with $I > 0$ may be called magnetic as they develop the magnetic fields along the axis of spins and give rise to the phenomenon of nuclear magnetic resonance. Such nuclei do not simply possess magnetic dipoles, but rather possess electric quadrupoles (it measures electric charge distribution within a nucleus when it possesses non-spherical symmetry) and interact with both, magnetic and electric gradients. The relative importance of the two effects is related to their magnetic moments and electric quadrupole moments.

1.2 Spinning nuclei in magnetic fields

A spinning nucleus generates a magnetic moment and when placed in an uniform magnetic field H it tends to align itself with the field. Unless the axis of the nuclear magneton is oriented exactly parallel or antiparallel to the magnetic field, a certain force is exerted by the applied field. Because the nucleus is spinning, the effect is that its rotational axis draws out a circle perpendicular to the external field (Fig. 1). This motion is called precession. The precessional angular velocity of a spinning top is known as Larmor frequency ω which is proportional to the applied field and can be expressed by Eq. (4) (the gyromagnetic ratio γ is equal to the ratio of the angular precessional frequency and the applied field) :

$$\omega = \gamma H . \quad (4)$$

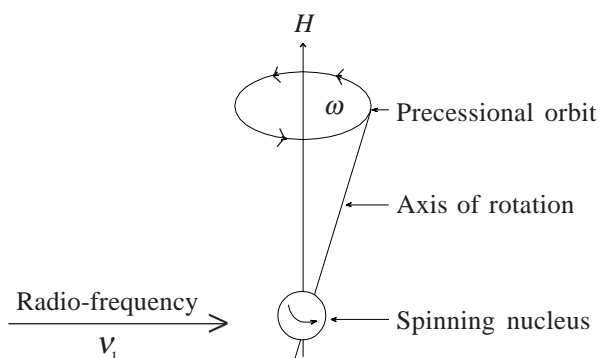


Fig. 1. Spinning nuclei in magnetic fields.

Table 1. Magnetic properties of NMR nuclei

Isotope	Natural abundance %	Spin number I	Magnetogyric ratio γ rad/G	Magnetic moment μ Bohr magneton	Electrical quadrupole moment $e \cdot 10^{-24} \text{ cm}^2$
$^1\text{H}_1$	99.9844	1/2	26753	2.79270	–
$^2\text{H}_1$	0.156	1	4107	0.85738	$2.77 \cdot 10^{-3}$
$^3\text{H}_1$	–	1/2	–	2.9788	–
$^{10}\text{B}_5$	18.83	3	–	1.8006	0.111
$^{11}\text{B}_5$	81.17	3/2	–	2.6880	$3.55 \cdot 10^{-2}$
$^{13}\text{C}_6$	1.108	1/2	6728	0.70216	–
$^{14}\text{N}_7$	99.635	1	–	0.40357	$2 \cdot 10^{-2}$
$^{15}\text{N}_7$	0.365	1/2	–2712	–0.28304	–
$^{17}\text{O}_8$	0.037	5/2	–3628	–1.8930	$-4 \cdot 10^{-3}$
$^{19}\text{F}_9$	100.00	1/2	25179	2.6273	–
$^{29}\text{Si}_{14}$	4.70	1/2	–5319	–0.55477	–
$^{31}\text{P}_{15}$	100.00	1/2	10840	1.1305	–
$^{33}\text{S}_{16}$	0.74	3/2	2054	0.64274	$-5.5 \cdot 10^{-2}$
$^{35}\text{S}_{16}$	–	3/2	–	1.00	$4.5 \cdot 10^{-2}$
$^{35}\text{Cl}_{17}$	75.40	3/2	2627	0.82089	$-7.97 \cdot 10^{-2}$
$^{37}\text{Cl}_{17}$	24.60	3/2	2184	0.68329	$-6.21 \cdot 10^{-2}$
$^{79}\text{Br}_{35}$	50.54	3/2	0.34	2.0991	–
$^{81}\text{Br}_{35}$	49.46	3/2	0.28	2.2626	–
$^{127}\text{I}_{53}$	100.00	5/2	0.75	2.7937	–
$^{183}\text{W}_{74}$	14.40	1/2	–	0.177	–

The precessional frequency ν can be expressed by Eq. (5) :

$$\frac{\omega}{2\pi} = \nu \text{ or } \omega = 2\pi\nu = \gamma H, \quad (5)$$

$$\nu = \frac{\gamma H}{2\pi}. \quad (6)$$

The Larmor frequency is such that a projection of the angular momentum on the direction H always assume whole multiple of $h/(2\pi)$ and as such, not all possible precession “cones” occur, only some selected ones. The number of these possible alignments are $2I + 1$ for spin I in the direction of magnetic field. These $2I + 1$ orientations are quantized in the direction of magnetic field and absorbable component m_1 of the spin I can be expressed by Eqs. (7) and (8) for half the integer (or integral number) and integer spins respectively :

$$m_1 = I, I-1, I-2 \dots 1/2, -1/2 \dots -(I-2), -(I-1), -I, \quad (7)$$

$$m_1 = I, I-1, I-2 \dots 1, 0, \dots -(I-1), -(I-2), -I. \quad (8)$$

In each case there are $2I + 1$ values of m_1 . Each orientation is associated with a different energy level E and can be expressed by Eq. (9) :

$$E = -\mu H \text{ or } E = -\frac{\gamma h}{2\pi} H m_1. \quad (9)$$

This type of splitting of energy levels in magnetic fields for a nucleus ($I > 0$) is called as nuclear zeeman splitting.

1.3 Theory of nuclear resonance

The basis of nuclear magnetic resonance is to induce transitions between the nuclear zeeman energy levels. Such transitions are affected by placing an alternating field H_1 perpendicular to the applied field H in such a way that frequency can be altered conveniently. Selection rules permit such transitions between energy levels for $m_2 - m_1 = \Delta_m = \pm 1$ i.e. $\Delta_m = +1$ when energy is absorbed (transition is from lower to higher energy level) and $\Delta_m = -1$ when energy is emitted (transition from higher to lower energy level). Such transitions from E_2 to E_1 energy levels can be expressed by Eq. (10) :

$$\Delta E = E_2 - E_1 = \frac{\gamma h}{2\pi} H m_2 - \frac{\gamma h}{2\pi} H m_1 = \frac{\gamma h}{2\pi} H (m_2 - m_1). \quad (10)$$

According to selection rules of quantum mechanics, $m_2 - m_1 = \pm 1$ depending on whether energy is absorbed or emitted, Eq. (10) is reduced to Eq. (11) :

$$\Delta E = \pm \frac{\gamma h H}{2\pi}. \quad (11)$$

When the frequency of electromagnetic radiation necessary to induce a transition from one nuclear spin state to another, is exactly equal to the precessional frequency of spinning nucleus, they are in resonance and the phenomenon of resonance occurs. Thus nuclear resonance (absorption or emission of energy) occurs when a magnetic nucleus ($I > 0$) is placed in an uniform magnetic field H and subjected to electromagnetic radiation of appropriate frequency matching to the precessional frequency of spinning. Under these conditions the frequency of electromagnetic radiation causing resonance can be expressed by Eq. (12) :

$$\Delta E = h \nu = \frac{\gamma h H}{2\pi}, \quad (12)$$

$$\text{or } \nu = \frac{\gamma H}{2\pi} \quad (12)$$

Eq. (12) also exhibits that the precessional frequency ν is $\frac{\gamma H}{2\pi}$.

Eq. (12) correlating electromagnetic frequency causing nuclear resonance with magnetic field strength is the basis of NMR spectroscopy and from this equation the electro-radiation frequency causing resonance for various field strengths can be calculated. Precessional frequencies for some nuclei at various field strengths are summarized in Table 2.

Table 2. Precessional frequencies as a function of field strength

	ν [MHz]						
H[kG] Nucleus	14	21	23	47	71	94	117
$^1\text{H}_1$	60.0	90.0	100.0	200.0	300.0	400.0	500.0
$^2\text{H}_1$	9.2	13.8	15.3	30.7	46.0	61.4	76.8
$^3\text{H}_1$	63.6	95.4	104.5	213.5	322.5	426.9	531.4
$^{10}\text{B}_5$	6.4	9.61	10.5	21.5	32.5	43.0	53.6
$^{11}\text{B}_5$	19.2	28.7	32.0	64.2	96.9	128.8	159.8
$^{13}\text{C}_6$	15.1	22.6	25.1	50.3	75.5	100.8	125.7
$^{14}\text{N}_7$	4.3	6.5	7.2	14.5	21.7	29.1	36.1
$^{15}\text{N}_7$	6.1	9.1	10.1	20.3	30.4	40.7	50.7
$^{17}\text{O}_8$	8.1	12.2	13.6	27.1	40.7	54.5	67.8
$^{19}\text{F}_9$	56.5	84.7	94.1	188.2	288.2	377.6	470.5
$^{29}\text{Si}_{14}$	11.8	17.8	19.5	39.8	60.1	79.5	99.0
$^{31}\text{P}_{15}$	24.3	36.4	40.5	81.0	121.5	162.8	202.0
$^{33}\text{S}_{16}$	4.6	6.9	7.5	15.4	23.2	30.7	38.2
$^{35}\text{S}_{16}$	7.1	10.7	11.7	23.9	36.1	47.8	59.5
$^{35}\text{Cl}_{17}$	5.8	8.7	9.6	19.6	29.6	39.2	48.8
$^{37}\text{Cl}_{17}$	6.9	10.3	11.3	23.0	34.7	46.0	57.3
$^{79}\text{Br}_{35}$	14.9	22.4	24.5	50.1	75.7	100.3	124.8
$^{81}\text{Br}_{35}$	16.1	24.2	26.5	54.0	81.6	108.1	134.5
$^{127}\text{I}_{53}$	11.9	17.9	19.6	40.0	60.5	80.1	99.7
$^{183}\text{W}_{74}$	2.5	3.67	4.0	8.2	12.4	16.5	20.5

1.4 Chemical shift

The fundamental NMR Eq. (12), $\nu = \frac{\gamma H}{2\pi}$, exhibits that a single peak should be obtained from the interaction of radiofrequency energy and the magnetic field on a nucleus as γ is characteristic for a nucleus. However the nucleus is shielded by an electron cloud whose density varies with the environment. This variation gives rise to different absorption positions. Under the influence of the applied magnetic field electrons circulate and generate their own magnetic field opposing the applied field and cause a shielding effect. The magnitude of the induced field is proportional to the magnetic

field. The effective magnetic field experienced by the nucleus is changed by this small local field σH (due to electronic circulation), such that H (effective) = $H - \sigma H$. A nucleus in different environments is shielded by the circulation of surrounding electrons to different extents. Different values of σH , each depending on the magnitude of the applied field H are obtained for the nucleus. Because the strength of the applied magnetic field cannot be determined to the required degree of accuracy, the absolute position of absorptions cannot be obtained directly from the instrument. However the relative position of absorption can readily be obtained with an accuracy of ± 1 Hz. The separation of resonance frequencies of a nucleus in different structural environments from some arbitrarily chosen standard is termed as chemical shift. A plot of the chemical shift (frequencies of absorption peaks) versus the intensities of absorption peaks which by integration provides the number of nuclei constitutes a NMR spectra. The chemical shift is symbolized by δ (delta) in ppm (parts per million) and is expressed by Eq. (13) :

$$\delta \text{ (ppm)} = \frac{H_S - H_R}{H_R} \cdot 10^6, \quad (13)$$

where H_S and H_R refer to the fields at resonance for sample s and reference substance r.

Since field and frequency are linearly related Eq. (13) can be transformed to Eq. (14) :

$$\delta \text{ (ppm)} = \frac{V_S - V_R}{V_R} \cdot 10^6, \quad (14)$$

where V_S and V_R are the resonance frequencies of sample s and reference r, respectively, in Hz.

The chemical shift in Hz is directly proportional to the applied field H and therefore to the applied frequency. It is dependent on diamagnetic shielding induced by the applied field. It is a ratio of the necessary change in field to the reference field or the necessary change in frequency to the standard reference frequency and hence a dimensionless number. To spread out chemical shifts i.e. to increase separation of resonance signal a high magnetic field is applied which constitutes high resolution NMR spectroscopy.

Chemical shifts are also expressed in an alternative scale τ (tau) which is related to δ (delta) by Eq. (15) :

$$\tau = 10.00 - \delta \quad (15)$$

High values of chemical shifts (δ ppm) correspond to high frequency shifts (down field or low field) due to deshielding; and low values correspond to low frequency shifts (upfield or high field) due to shielding.

1.5 Coupling constant

The position of the resonance signal of a nucleus A depends on its magnetic environment : part of its magnetic environment is the nearby nucleus B which itself is magnetic and nucleus B can either have its nuclear magnet aligned with nucleus A or opposed to nucleus A. In this way nucleus B can either increase the net magnetic field experienced by nucleus A (B aligned) or decrease it (B opposed); in fact it does both. The two spin orientations of B creates two different magnetic fields around nuclei A. As such nuclei A comes to resonance twice and gives rise to a doublet in NMR spectrum. Similarly nucleus A is magnetic having two spin orientations and creates two magnetic fields

around nucleus B. Nucleus B comes to resonance twice and gives rise to a doublet in NMR spectrum. The mutual magnetic influence between nuclei A and B is transmitted via the electrons in the intervening bonds (not through space). The electron-coupled spin interaction operates strongly through one or two bonds, less strongly through three bonds and weakly through more bonds. A signal can split into a doublet or multiplet depending upon the number of interacting neighbour nuclei. Splitting of the spectral lines arises due to coupling interactions between neighbour nuclei and is related to the number of possible orientations that neighbour nuclei can adopt. Splitting arises because of spin-spin interactions or coupling and this phenomenon is known as spin-spin splitting or spin-spin coupling. Spin-spin splitting (separation of a resonance signal) is expressed in terms of the coupling constant J . It is a measure of the interaction of nuclei interacting through intervening electrons. It is independent of applied magnetic field and is expressed in units of frequency (Hz). Generally, J is expressed as, $^1J_{AB}$, $^2J_{AB}$... to indicate that nuclei A and B are interacting through 1, 2, 3... bonds.

1.6 Organization of data

This volume contains chemical shifts δ (in ppm) and coupling constants J (in Hz) for hydrogen-1 nuclei. For hydrogen-1 nuclei the arrangement of compounds is based on their gross formulae arranged according to Hill's system i.e. in alphabetical order of elements except for compounds containing carbon. Compounds which contain carbon have been arranged considering carbon and hydrogen on priority in ascending order followed by alphabetical arrangement for other atoms present in the molecule. Chapter 2 deal with NMR data for ^1H . Sections 2.1, 2.2, 2.3 (chapter 2) dealing with chemical shifts are printed in this subvolume. Sections 2.4 and 2.5 of chapter 2 dealing with coupling constants are only provided on the CD-ROM included in this book. Additionally all data printed in this subvolume are also provided on the CD-ROM.

2 Hydrogen-1 NMR

2.1 Introduction for 2

Hydrogen nucleus is the simplest one and ^1H is naturally occurring isotope (99.98 abundance) with spin number $I = \frac{1}{2}$ and magnetic moment $\mu = 2.7927$ nuclear magnetons. Hydrogen-1 is the nucleus on which phenomenon of nuclear magnetic resonance (NMR) was first time observed in 1946. The magnetic moment of ^1H is fairly large and detection of pmr spectra is fairly sensitive. In a magnetic field of 21 KG the resonance frequency for ^1H is 90 MHz and the chemical shift extends over a range of 0–15 ppm. Hydrogen-1 nmr spectra are commonly screened at 60,80,90 and 100 MHz corresponding to magnetic fields of 14092, 18667, 21000 or 23500 gauss respectively. Higher frequencies (up to 500 MHz) are used in conjunction with superconducting helium-cooled magnets. ^1H NMR spectroscopy has emerged as one of the most useful and reliable technique for the determination of molecular structure and bonding, to study isomerism, substituent effects, rate of proton exchange, activation energy etc., and for diagnostic purposes in biomedical investigations. ^1H NMR (proton magnetic resonance, pmr) spectra for a vast variety of compounds of almost all series have been extensively studied.

This subvolume includes enormous amount of Hydrogen-1 NMR data of organic compounds except on heterocycles and natural products which will be covered in subvolumes III/35C,Part-2 and Part-3 respectively. Chemical shifts δ (in ppm) and coupling constants $^nJ(\text{HX})$ (in Hz) have been organized by arranging the gross formulae according to Hill's system as explained in the introduction (section 1.6). Chemical shifts (in ppm) are expressed relative to the signal of tetramethylsilane (TMS) as an internal standard. The prefix n in nJ indicates the number of bonds over which coupling is occurring.

ABBREVIATIONS

Me	–	Methyl	Bu ^t	–	Tertiarybutyl
Et	–	Ethyl	c-C ₆ H ₁₁	–	Cyclohexyl
Pr ⁿ	–	Normalpropyl	Ph	–	Phenyl
Pr ⁱ	–	Isopropyl	DMSO	–	Dimethyl sulfoxide
Bu ⁿ	–	Normalbutyl	TFA	–	Trifluoroacetic acid
Bu ⁱ	–	Isobutyl	THF	–	Tetrahydrofuran
Bu ^s	–	Secondarybutyl			

2.2 Table for ^1H chemical shift δ , downfield from tetramethylsilane (TMS). All measurements refer to room temperature if not stated otherwise.

No.	Gross formula	Solvent	δ [ppm]	Ref.
1	$\text{C}_2\text{H}_2\text{ClFO}$	SO_2 -70°C	4.89(a,2H)	75Ola
2	$\text{C}_2\text{H}_3\text{ClF}_2$	–	3.82(a,2H),6.11(b)	72Ola
3	$\text{C}_2\text{H}_3\text{FO}$	SO_2 -70°C	2.07(a,3H)	75Ola
4	$\text{C}_2\text{H}_4\text{F}_2$	–	1.78(a,3H),5.9(b)	72Ola
5	$\text{C}_2\text{H}_4\text{F}_2\text{O}_3\text{S}$	–	1.84(a,3H),6.42(b)	72Ola
6	C_3HBrF_6	CDCl_3	4.5(a)	89Han1
7	C_3HClF_6	CDCl_3	4.52(a)	89Han1
8	$\text{C}_3\text{HCl}_2\text{F}_3\text{O}$	CDCl_3	9.3(a)	85Mar
9	$\text{C}_3\text{H}_2\text{ClF}_3\text{O}_2$	CDCl_3	4.73(a),10.3(b)	87Bla
10	$\text{C}_3\text{H}_2\text{IN}$	CCl_4	7.63(a),6.75(b)	92Ma
11	$\text{C}_3\text{H}_3\text{Br}_2\text{FO}$	CDCl_3	4.0–4.5(a,2H),9.3(b)	85Mol2
12	$\text{C}_3\text{H}_3\text{F}_6\text{IO}_4\text{S}$	CDCl_3	4.93(a,2H),3.9(b)	96Zhd
13	$\text{C}_3\text{H}_4\text{BrNO}_2$	$\text{DMSO}-d_6$	4.5(a,2H),7.63(b),12.75(c)	73Tay
14	$\text{C}_3\text{H}_4\text{ClF}_3$	CDCl_3	1.63(a,3H),4.2(b)	89Han1
15	$\text{C}_3\text{H}_4\text{ClNO}_3\text{S}$	CDCl_3	4.0(a,4H)	76Kri
16	$\text{C}_3\text{H}_4\text{F}_2\text{O}$	CCl_4	5.58(a),3.58(b,3H)	83Whe
17	$\text{C}_3\text{H}_4\text{F}_3\text{I}$	CDCl_3	1.94(a,3H),4.16(b)	89Han1
18	$\text{C}_3\text{H}_5\text{BrFNO}_3$	CDCl_3	3.25(a),3.92(b,2H),3.85(c,2H)	80Ber
19	$\text{C}_3\text{H}_5\text{ClF}_3\text{NO}_2$	CD_3OD	5.04(a)	97Sol
20	$\text{C}_3\text{H}_5\text{NO}_3$	CDCl_3	3.12(a,2H),4.66(b,2H),9.6(c)	86Öhr
21	$\text{C}_3\text{H}_5\text{NS}$	CCl_4	2.9(a,2H),1.5(b,3H)	79Kat
22	$\text{C}_3\text{H}_6\text{BrF}$	CDCl_3	2.4(a,4H),4.0(b,2H)	86Pat
23	$\text{C}_3\text{H}_6\text{F}_6\text{N}_4$	CCl_4	4.57(a,6H)	70Din
24	$\text{C}_3\text{H}_6\text{N}_2\text{O}_3$	CDCl_3	3.7(a,3H),7.2(b,2H),9.9(c)	88Por
25	$\text{C}_3\text{H}_7\text{BrO}$	CDCl_3	1.67(a,3H),3.07(b),3.75(c,2H),4.25(d)	76Arm
26	$\text{C}_3\text{H}_7\text{ClOS}$	CDCl_3	1.6(a),2.77(b,2H),3.4(c),3.7(d,2H),3.6–4.15(e)	86Mat
27	$\text{C}_3\text{H}_7\text{F}$	CDCl_3	1.4(a,6H),4.83(b)	86Pat
28	$\text{C}_3\text{H}_7\text{NOS}$	CDCl_3	2.26(a,3H),2.83(b,3H),5.2(c)	93Tan
29	$\text{C}_3\text{H}_7\text{NOS}$	CDCl_3 37°C	2.38(a,3H),2.1(b,3H),6.5(c)	72Kis
30	$\text{C}_3\text{H}_8\text{ClN}$	CDCl_3	1.21(a,3H),2.85(b,3H),2.92(c,2H)	88Gui
31	$\text{C}_3\text{H}_{12}\text{Cl}_2\text{N}_2$	D_2O	1.68(a,3H),3.25(b,3H),3.25(c,2H)	81Klu
32	$\text{C}_4\text{HF}_3\text{O}$	–	3.21(a)	85She
33	$\text{C}_4\text{H}_2\text{F}_6\text{OS}_2$	CDCl_3	5.15(a),9.5(b)	98Kol
34	$\text{C}_4\text{H}_3\text{ClF}_2$	CDCl_3	2.66(a,2H),6.3(b)	87Dol1
35	$\text{C}_4\text{H}_3\text{Cl}_3$	CCl_4	5.35(a,2H),6.1(b)	85Rus
36	$\text{C}_4\text{H}_3\text{F}_8\text{IO}_4\text{S}$	CDCl_3	6.02(a),4.93(b,2H)	96Zhd

No.	Gross formula	Solvent	δ [ppm]	Ref.
37	C ₄ H ₄ Br ₄	–	2.1(a),1.36(b,3H)	94Dul
38	C ₄ H ₄ ClFO ₂	CDCl ₃	7.33(a),4.04(b,3H)	96Shi2
39	C ₄ H ₄ F ₂	CDCl ₃	1.36(a,4H)	86Dol
40	C ₄ H ₅ BrS	CCl ₄	2.78(a,2H),1.4(b,3H)	80Com
41	C ₄ H ₅ Cl ₃ O	CDCl ₃	4.98(a),2.45(b),1.32(c,3H)	91Kru
42	C ₄ H ₅ Cl ₃ O	CDCl ₃	4.0(a,2H),4.95(b),6.25(c)	81Mac
43	C ₄ H ₅ F	CDCl ₃	6.88(a),1.27(b,4H)	83Dol2
44	C ₄ H ₅ FO ₃	CDCl ₃	9.87(a),7.03(b),3.95(c,3H)	96Shi2
45	C ₄ H ₅ FO ₃	D ₂ O	1.36(a,3H),4.86(b)	91Res
46	C ₄ H ₅ F ₃ O	–	3.7(a,3H),4.58(b),6.21(c)	71Rau
47	C ₄ H ₅ F ₃ O ₂	CCl ₄	1.39(a,3H),4.33(b,2H)	87For
48	C ₄ H ₅ F ₄ NO ₆ S	CDCl ₃	2.65(a),4.1(b,2H),5.07(c,2H)	80Ber
49	C ₄ H ₅ F ₆ N	CDCl ₃	1.7(a,2H),1.46(b,3H)	95Buc
50	C ₄ H ₆ BrFO ₂	CDCl ₃	1.36(a,3H),4.4(b,2H),6.64(c)	89Elk
51	C ₄ H ₆ BrN	CDCl ₃	1.44(a,3H),3.1(b),3.45(c,2H)	87Mur1
52	C ₄ H ₆ Cl ₂	CDCl ₃	4.12(a,4H),5.7–5.95(b,2H)	93Alt
53	C ₄ H ₆ FN ₃ O ₂	CDCl ₃	1.4(a,3H),4.33(b,2H),5.44(c)	88Tak
54	C ₄ H ₆ F ₂	CCl ₄	4.97(a,4H),5.53–6.1(b,2H)	84She1
55	C ₄ H ₆ F ₂ I ₂	CDCl ₃	2.98(a,3H),2.12(b,3H)	86Roz
56	C ₄ H ₆ O	–	3.2(a,2H),5.3(b),5.7–6.0(c,2H),9.7(d)	98Cri
57	C ₄ H ₆ O ₂	CCl ₄	1.1(a,3H),2.27(b,2H),9.08(c)	82Ver
58	C ₄ H ₆ O ₂ S	CCl ₄	1.34(a,3H),3.0(b,2H),9.2(c)	73And
59	C ₄ H ₇ BrO	CCl ₄	3.55(a,3H),3.79(b,2H),4.03(c),4.23(d)	77Jac
60	C ₄ H ₇ BrO	CDCl ₃	9.8(a),3.45(b,2H),2.6(c,2H),2.2(d,2H)	82Lit
61	C ₄ H ₇ BrO	CDCl ₃	6.76(a),5.37(b),3.78(c,2H),1.31(d,3H)	97Sch
62	C ₄ H ₇ BrO ₂	CCl ₄	1.8(a,3H),3.74(b,3H),4.29(c)	78Oga
63	C ₄ H ₇ ClOS	–	5.51(a),1.44(b,6H)	86Sch
64	C ₄ H ₇ Cl ₂ NO ₃	CDCl ₃	1.12(a,3H),1.62(b,2H),4.89(c),5.78(d)	94Dem
65	C ₄ H ₇ FO	CCl ₄	4.68(a,2H),2.61(b,2H),1.2(c,3H)	88Wel
66	C ₄ H ₇ FO	CDCl ₃	2.1(a,3H),2.7(b,2H),4.67(c,2H)	86Pat
67	C ₄ H ₇ F ₃ O ₃ S	CDCl ₃	1.03(a,3H),1.78(b,2H),4.48(c,2H)	85Aub
68	C ₄ H ₇ IO	CDCl ₃	5.98(a),4.21(b,2H),2.92(c),1.7(d,3H)	82Ens
69	C ₄ H ₇ IO ₂	CCl ₄	1.93(a,3H),3.7(b,3H),4.43(c)	80Oga

No.	Gross formula	Solvent	δ [ppm]	Ref.
70	C ₄ H ₇ N	CDCl ₃	1.4(a),2.32(b),2.47(c,3H),3.38(d,2H)	88Mas
71	C ₄ H ₇ N	CDCl ₃	1.1(a,3H),1.7(b,2H),2.53(c,2H)	85Ors
72	C ₄ H ₇ NO ₂	CDCl ₃	2.17(a,3H),4.19(b,2H),8.37(c)	90Yin
73	C ₄ H ₇ NO ₂	CDCl ₃	1.21(a,3H),2.47(b,2H),9.12(c),9.48(d)	80Lin
74	C ₄ H ₇ NO ₃	CCl ₄	2.05(a,3H),4.57(b,2H),7.37(c)	74Aue
75	C ₄ H ₇ NS	CCl ₄	2.9(a,2H),1.1(b,3H),1.5–2.2(c,2H)	79Kat
76	C ₄ H ₇ N ₃ O	DMSO-d ₆	7.04&7.05(a,2H),3.63(b,2H),3.14(c,2H),2.81(d)	83Kaw
77	C ₄ H ₈ Cl ₂ O	CDCl ₃	2.45(a,2H),3.55(b,3H),3.7(c,2H),5.65(d)	90Sal
78	C ₄ H ₈ I ₂ O ₂	CDCl ₃	2.56(a,2H),3.33(b,4H),3.93(c,2H)	97Som
79	C ₄ H ₈ N ₂ O	CCl ₄	6.66&6.34(a,2H),3.13(b,3H),2.22(c,3H)	72Con
80	C ₄ H ₈ N ₂ O ₂	CDCl ₃	1.37(a,3H),4.06(b,2H),3.9(c,3H)	71Tsu
81	C ₄ H ₈ O	CCl ₄	4.46(a),4.18(b),0.8–2.5(c,6H)	83Fad
82	C ₄ H ₈ O ₂	CCl ₄	3.1(a),3.48(b,3H),3.93(c,2H),4.83(d),6.42(e)	80Ire
83	C ₄ H ₈ O ₂	–	2.2(a,3H),4.25(b),1.39(c,3H)	91Cro
84	C ₄ H ₈ O ₂ S	CDCl ₃	1.47(a),2.07(b,3H),2.74(c,2H),4.18(d,2H)	98Li
85	C ₄ H ₈ O ₃	CDCl ₃	1.91(a,3H),2.26(b,2H),3.2–3.5(c,2H),3.97(d)	92Kob
86	C ₄ H ₈ O ₄ S	CDCl ₃	1.2(a,3H),2.58(b,2H),3.26(c,3H)	71Kar1
87	C ₄ H ₉ ClO	Neat	0.9(a,3H),1.9(b),3.5(c,2H),3.6(d,2H),4.6(e)	75Kab
88	C ₄ H ₉ N	CDCl ₃	1.3(a),2.4(b,3H),3.27(c,2H),5.26(d,2H),5.67(e)	88Mas
89	C ₄ H ₉ N	CDCl ₃	1.16(a,3H),1.9(b,3H),3.33(c,2H),7.63(d)	93Ste
90	C ₄ H ₉ NOS	CDCl ₃ 37°C	1.26(a,3H),2.16(b,3H),2.77(c,2H),7.59(d)	72Kis
91	C ₄ H ₉ NOS	CDCl ₃	1.28(a,3H),2.82(b,3H),2.93(c,2H)	93Tan
92	C ₄ H ₉ NOS	CDCl ₃	2.02(a,3H),2.85(b,2H),3.55(c,2H),6.42(d)	85Bew2
93	C ₄ H ₉ NO ₂	CDCl ₃	0.95(a,6H),2.38(b),4.17(c,2H)	78Bor
94	C ₄ H ₉ NO ₂	CDCl ₃	1.29(a,3H),1.99(b,3H),4.01(c,2H)	85Joh
95	C ₄ H ₉ N ₃ OS	CDCl ₃	1.37(a,3H),3.46(b,3H),3.56–4.02(c,2H),8.58(d)	85Iso
96	C ₄ H ₁₀ ClN	CDCl ₃	1.15(a,6H),2.91(b,3H),3.05(c)	88Gui
97	C ₄ H ₁₀ ClNO ₂	D ₂ O	2.78(a,2H),3.82(b,2H),4.05(c,2H)	84Fin
98	C ₄ H ₁₀ ClNO ₂ S	CDCl ₃	1.3(a,6H),3.4(b,4H)	77Gup
99	C ₄ H ₁₀ N ₂ O ₂	D ₂ O	7.32&6.78(a),4.84(b,3H),4.28&4.18(c,2H), 3.72(d,2H),3.19(e,2H)	77Nie
100	C ₄ H ₁₀ O ₃	D ₂ O	3.65(a,4H),1.2(b,4H)	84Cop
101	C ₄ H ₁₀ S ₂	CCl ₄	1.32(a,6H),2.66(b,4H)	78Aki

No.	Gross formula	Solvent	δ [ppm]	Ref.
102	C ₄ H ₁₁ NO	CDCl ₃	1.1(a,3H),1.4–1.67(b,2H),3.07(c),3.55(d,3H), 3.62–3.83(e,2H)	94Bar2
103	C ₄ H ₁₂ N ₂ O ₂	D ₂ O	4.88(a,4H),3.7(b,4H),2.9(c,4H)	77Nie
104	C ₄ HF ₁₁	–	3.32(a)	79Has
105	C ₅ H ₃ ClF ₂ O ₂	CDCl ₃	3.2(a,2H),11.0(b)	87Dol1
106	C ₅ H ₃ Cl ₂ F ₃	CDCl ₃	6.65(a),3.32(b,2H)	84Dol
107	C ₅ H ₃ Cl ₃ F ₂	CDCl ₃	3.47(a,2H),6.35(b)	86Pas
108	C ₅ H ₃ F ₃ O ₂	CCl ₄	4.48(a,3H)	76Sma
109	C ₅ H ₃ F ₇ OS	CCl ₄	2.3(a,3H)	86Kre2
110	C ₅ H ₄ F ₄	CCl ₄	6.45(a),1.92(b,3H)	83Dol1
111	C ₅ H ₄ F ₅ N ₃	CCl ₄	3.93(a,2H),6.33(b),5.85(c)	78Man
112	C ₅ H ₄ F ₆ O	–	3.9(a,3H),5.66(b)	71Rau
113	C ₅ H ₅ BrO ₃	CDCl ₃	9.38(a),7.42(b),3.89(c,3H)	77Far
114	C ₅ H ₅ ClF ₄	Neat	2.9(a,2H),5.1–6.0(b,3H)	91Hu
115	C ₅ H ₅ F ₃ N ₂ O ₂	CCl ₄	1.25(a,3H),4.2(b,2H)	90Shi1
116	C ₅ H ₅ F ₃ O ₂	CDCl ₃	4.5(a,2H),1.4(b,3H)	90Tor
117	C ₅ H ₅ F ₇ S	–	2.95(a,2H),1.35(b,3H)	72Has
118	C ₅ H ₅ NO ₃	CDCl ₃	4.5(a,2H),1.38(b,3H)	82Ach
119	C ₅ H ₆	CCl ₄	1.4(a,4H),4.65(b,2H)	77Den
120	C ₅ H ₆ BrFO	CDCl ₃	5.55(a),4.45(b),2.5–3.2(c,4H)	85Roz
121	C ₅ H ₆ ClF ₃ O	CDCl ₃	3.0(a,2H),3.45(b,2H),3.75(c,2H)	80Mol
122	C ₅ H ₆ Cl ₂ O	CCl ₄	1.43(a,3H),1.9–2.25(b,2H),9.95(c)	77Khu1
123	C ₅ H ₆ Cl ₂ O ₃	CDCl ₃	7.42(a),4.21(b,2H),1.36(c,3H)	90Bow
124	C ₅ H ₆ F ₄	CDCl ₃	1.07(a,3H),2.23(b,2H),5.54(c)	87Dol2
125	C ₅ H ₆ F ₄ O ₂	–	1.35(a,3H),4.38(b,2H),5.11(c)	93Muz1
126	C ₅ H ₆ I ₂ O ₂	CDCl ₃	7.62(a),4.28(b,2H),1.35(c,3H)	79Hol1
127	C ₅ H ₆ O	CDCl ₃	2.0(a,3H),2.27(b,3H)	70Byr
128	C ₅ H ₆ O	CCl ₄	5.67(a),5.17(b,2H),2.25(c,3H)	82Fle
129	C ₅ H ₆ O	CDCl ₃	1.68–1.71(a,2H),2.24–2.29(b),5.49–5.54(c,2H), 8.5(d)	94Cor1
130	C ₅ H ₇ Br	CCl ₄	5.95(a),3.8(b,2H),2.0–2.95(c,4H)	71She
131	C ₅ H ₇ Cl	CDCl ₃	1.13(a,3H),2.23(b,2H),4.11(c,2H)	70Byr
132	C ₅ H ₇ ClO	CCl ₄	1.42(a,4H),2.46(b,3H)	77Fit1

No.	Gross formula	Solvent	δ [ppm]	Ref.
133	C ₅ H ₇ ClO	CDCl ₃	1.03(a,3H),2.45(b,2H),7.13(c),9.47(d)	82Bar
134	C ₅ H ₇ ClO	CDCl ₃	6.4(a),2.52(b,3H),2.2(c,3H)	80Bar3
135	C ₅ H ₇ Cl ₃ O ₂ S ₃	–	4.71(a),1.4(b,6H)	86Sch
136	C ₅ H ₇ FO	CCl ₄	1.05–1.45(a,4H),2.47(b,3H)	77Fit1
137	C ₅ H ₇ FO	CDCl ₃	1.15(a,3H),2.3(b,2H),5.98(c),9.21(d)	84Cam
138	C ₅ H ₇ FO ₄	–	1.34(a,3H),4.34(b,2H),5.4(c),10.2(d)	86Kit
139	C ₅ H ₇ FO ₄	CDCl ₃	5.33(a),3.38(b,6H)	83Ler
140	C ₅ H ₇ F ₃ O ₂	SO ₂ –70°C	5.05(a),1.17(b,6H)	75Ola
141	C ₅ H ₇ F ₃ O ₃ S	–	1.11(a,3H),3.92(b,2H),5.82(c),7.35(d)	98Zhu
142	C ₅ H ₇ F ₄ NO ₂	CD ₃ OD	2.42–3.03(a,2H),4.55(b),6.14(c)	96Sol
143	C ₅ H ₇ I	CCl ₄	4.82–5.35(a),4.5–4.82(b,2H),3.15(c,2H), 2.15–2.92(d,2H)	71She
144	C ₅ H ₇ NO	CDCl ₃	1.5(a,3H),2.4(b,3H),3.7(c)	89Ito
145	C ₅ H ₇ NO	CDCl ₃	2.03(a,3H),3.7(b,3H),6.45(c)	86Hof1
146	C ₅ H ₇ NO ₂	CDCl ₃	2.1(a,3H),2.65(b,2H),3.35(c,2H)	79Hei
147	C ₅ H ₇ NO ₃	CDCl ₃	1.36(a,3H),4.33(b,2H),4.8(c,2H)	76Din
148	C ₅ H ₇ N ₃ O ₅	CDCl ₃	2.06(a,2H),2.82(b,2H),3.07(c,2H),8.28(d)	98Smi
149	C ₅ H ₈ BrN ₃	CDCl ₃	1.1(a,3H),2.25(b,2H),4.05(c,2H),6.1(d)	86Has
150	C ₅ H ₈ ClFO	CDCl ₃	1.24(a,3H),1.1–1.9(b,2H),2.3–2.9(c,3H)	84Cam
151	C ₅ H ₈ ClO	CCl ₄	1.38(a,3H),2.54(b),4.17(c,2H),4.3(d),6.0(e)	77Sey
152	C ₅ H ₈ Cl ₄	CCl ₄	1.87(a,6H),3.39(b,2H)	76Nak
153	C ₅ H ₈ FIO ₂	CDCl ₃	4.3–5.0(a,3H),4.2(b,2H),1.3(c,3H)	91Bar
154	C ₅ H ₈ IN ₃ O ₂	–	2.1(a,3H),3.83(b,3H),3.93(c,2H)	82Cam2
155	C ₅ H ₈ N ₂ O ₄	CDCl ₃	5.36(a),2.82(b,3H),1.35(c,3H)	94Pai
156	C ₅ H ₈ O	CCl ₄	1.05(a,3H),1.6(b,3H),2.0(c,2H)	80Mus
157	C ₅ H ₈ O	CDCl ₃	1.81(a,3H),4.46(b),1.4(c,3H),2.6(d)	70Byr
158	C ₅ H ₈ O	CDCl ₃	1.3–3.5(a,5H),1.15(b,3H)	80Was
159	C ₅ H ₈ O	CDCl ₃	5.22(a),4.81(b,2H),3.79(c,2H),2.37(d,2H),1.8(e)	93Rus
160	C ₅ H ₈ OS ₂	CDCl ₃	2.44(a,3H),2.55(b,3H),5.99(c),9.92(d)	88Die
161	C ₅ H ₈ O ₂	CDCl ₃	4.6(a),3.58(b),2.0–2.5(c,6H)	72McI
162	C ₅ H ₈ O ₂	CDCl ₃	6.34(a),5.82(b),3.72(c,3H),2.22(d,3H)	85Alc
163	C ₅ H ₈ O ₂	CDCl ₃	1.3(a,3H),4.21(b,2H),5.76–6.44(c,3H)	92Kow

No.	Gross formula	Solvent	δ [ppm]	Ref.
164	C ₄ H ₈ O ₂	CCl ₄	0.95(a,3H),1.3–1.95(b,2H),2.62(c,2H),9.0(d)	82Ver
165	C ₅ H ₈ O ₂ S ₂	CCl ₄	1.55(a,6H),4.76(b,2H)	72Sch
166	C ₅ H ₈ O ₃	CDCl ₃	2.59(a,2H),2.76(b,2H),3.7(c,3H),9.88(d)	88Gan
167	C ₅ H ₈ O ₃ S ₃	CDCl ₃	11.87(a),4.68(b,2H),4.0(c,2H),1.43(d,3H)	76Bar
168	C ₅ H ₈ O ₄	FSO ₃ H 37°C	4.35(a,6H),4.1(b,2H)	75Lar
169	C ₅ H ₈ O ₄	CD ₃ COCD ₃	6.2(a,2H),4.21(b,2H),2.72(c,2H),2.62(d,2H)	95Cot
170	C ₅ H ₈ S	CCl ₄	1.23(a,3H),2.04(b),2.6(c,2H),3.12(d,2H)	75Nis
171	C ₅ H ₉ BrO	CDCl ₃	1.4–2.5(a,6H),3.25(b),3.63(c,2H)	71Eri1
172	C ₅ H ₉ BrO	CCl ₄	3.6(a,2H),1.15(b,7H)	85Gad
173	C ₅ H ₉ BrO	CDCl ₃	9.2(a),3.5(b,2H),2.6(c,2H),1.99(d,4H)	82Lit
174	C ₅ H ₉ BrO ₂	CCl ₄	1.02(a,3H),2.04(b,2H),3.74(c,3H),4.08(d)	78Oga
175	C ₅ H ₉ BrO ₂	CCl ₄	1.9(a,6H),3.76(b,3H)	78Arn
176	C ₅ H ₉ ClF ₃ NO ₂	CD ₃ OD	1.29(a,3H),4.19(b,2H),5.31(c)	97Sol
177	C ₅ H ₉ ClO ₂	CCl ₄	3.68(a,3H),4.2(b),1.92(c,2H),1.0(d,3H)	75Oga
178	C ₅ H ₉ ClO ₂	CDCl ₃	1.0(a,3H),1.16–2.33(b,4H),6.53(c),8.06(d)	82Bar
179	C ₅ H ₉ ClO ₂ S	CDCl ₃	1.6(a),2.1(b,3H),2.8(c,2H),3.76(d,2H),5.0(e)	86Mat
180	C ₅ H ₉ Cl ₂ NO ₃	CDCl ₃	1.13(a,3H),1.41–1.72(b,4H),4.48(c),5.91(d)	94Dem
181	C ₅ H ₉ Cl ₃ O	CCl ₄	5.73(a),3.45–4.0(b,5H),1.41(c,3H)	70Sey
182	C ₅ H ₉ DO	CDCl ₃	3.7(a,2H),3.6(b,3H),2.6(c),2.1(d),1.7–2.0(e,2H)	89Gut
183	C ₅ H ₉ FO ₂ S	CDCl ₃	1.33(a,3H),2.77(b,2H),3.85(c,3H),5.95(d)	98Jou
184	C ₅ H ₉ F ₃ O ₂	CDCl ₃	1.23(a,3H),3.55–3.72(b,4H),3.85(c),4.1–4.2(d)	95Ram
185	C ₅ H ₉ F ₃ O ₃ S	CDCl ₃	0.95(a,3H),1.66(b,4H),4.48(c,2H)	85Aub
186	C ₅ H ₉ IO ₂	CCl ₄	0.97(a,3H),1.97(b,2H),3.71(c,3H),4.2(d)	80Oga
187	C ₅ H ₉ N	CDCl ₃	1.1(a,3H),1.45(b),2.2(c),2.62(d,2H),3.35(e,2H)	88Mas
188	C ₅ H ₉ NO ₂	CDCl ₃	2.25(a,3H),2.8(b,3H),3.35(c,2H)	92Sin
189	C ₅ H ₉ NO ₂ S	CDCl ₃	3.19(a,2H),2.26(b,2H),2.65(c,2H),2.97(d,3H)	72Dil
190	C ₅ H ₉ NO ₃	CDCl ₃	1.6(a,3H),2.15–2.61(b,2H),4.1–4.5(c,2H), 4.9–5.6(d,2H)	84Hru
191	C ₅ H ₉ NO ₃	CDCl ₃	8.22(a),7.0(b),4.1(c,2H),4.02(d,2H),1.25(e,3H)	91Nev
192	C ₅ H ₉ NO ₄	CDCl ₃	0.98(a,3H),1.48(b,3H),3.98(c,2H),4.9(d)	93Niy
193	C ₅ H ₉ NS	CCl ₄	2.9(a,2H),1.1–2.1(b,4H),0.8–1.1(c,3H)	79Kat
194	C ₅ H ₁₀	CD ₂ Cl ₂	5.75(a),4.89(b,2H),2.3(c),1.0(d,6H)	89Fle
195	C ₅ H ₁₀ BrF	CDCl ₃	1.52(a,3H),1.48(b,3H),1.7(c,3H),4.13(d)	89Cam
196	C ₅ H ₁₀ ClNO ₂	CDCl ₃	1.19(a,6H),3.87(b),4.85(c),5.75(d,2H)	96Pat

No.	Gross formula	Solvent	δ [ppm]	Ref.
197	C ₅ H ₁₀ ClNO ₂	CD ₃ COCD ₃	6.2&6.05(a),4.2(b,2H),3.0(c),1.7&1.68(d,6H)	85Al-H
198	C ₅ H ₁₀ ClN ₃ O	CDCl ₃	2.45(a,3H),3.23(b,3H),3.9(c,2H),4.12(d,2H)	88Smi
199	C ₅ H ₁₀ Cl ₂ O	Neat	5.8(a),3.6(b,3H),1.2(c,6H)	70Sey
200	C ₅ H ₁₀ Cl ₂ O	CDCl ₃	0.95(a,3H),1.65(b,2H),2.3(c),3.4-3.7(d,4H)	96Tan
201	C ₅ H ₁₀ DNOS	CCl ₄	1.23(a,3H),2.74(b),2.9(c,6H)	82Bea1
202	C ₅ H ₁₀ N ₂ O ₄	CDCl ₃	2.61(a,4H),1.06(b,6H)	92Asa
203	C ₅ H ₁₀ N ₆	CDCl ₃	0.91(a,6H),1.43(b,3H),1.8-2.0(c)	88Nis
204	C ₅ H ₁₀ O	CDCl ₃	0.1-1.1(a,5H),1.25(b,3H),2.6(c),3.0(d)	84Hru
205	C ₅ H ₁₀ O	CDCl ₃	5.0(a),4.86(b),4.08(c,2H),2.07(d,2H),1.63(e), 1.08(f,3H)	97Org
206	C ₅ H ₁₀ OS ₃	CCl ₄	4.36(a,2H),3.26(b,2H),2.65(c,3H),1.36(d,3H)	84Yok
207	C ₅ H ₁₀ O ₂	CDCl ₃	1.2(a,3H),2.18(b,3H),2.58(c,2H),3.35(d),4.22(e)	84Car1
208	C ₅ H ₁₀ O ₂	CDCl ₃	0.94(a,3H),1.1-1.9(b,4H),2.39(c,2H),10.5(d)	83Tak
209	C ₅ H ₁₀ O ₂	-	2.19(a,3H),4.17(b),0.94(c,3H),1.8(d,2H)	91Cro
210	C ₅ H ₁₀ O ₂ S	CCl ₄	4.1(a,2H),3.06(b,2H),2.19(c,3H),1.29(d,3H)	79Tan
211	C ₅ H ₁₀ O ₃	-	1.35(a,3H),3.32(b,3H),3.68(c,3H),3.74(d)	82Bec
212	C ₅ H ₁₀ O ₃	CDCl ₃	1.17(a,3H),2.47-3.03(b),3.33(c,3H),3.4-3.6(d,2H)	84Gri1
213	C ₅ H ₁₀ O ₃	CDCl ₃	1.6-1.8(a,2H),2.07(b,3H),2.08-2.22(c), 3.71(d,2H),4.24(e,2H)	96Hou
214	C ₅ H ₁₀ S ₃	CCl ₄	3.9(a,2H),3.23(b,2H),2.2(c,3H),1.37(d,3H)	84Yok
215	C ₅ H ₁₁ ClN ₄ O	CDCl ₃	2.95(a,3H),3.26(b,3H),3.86(c,2H),4.05(d,2H), 6.37(e)	88Smi
216	C ₅ H ₁₁ N	CDCl ₃	7.37(a,2H),1.17(b,9H)	74Mur
217	C ₅ H ₁₁ N	CDCl ₃	1.13(a,3H),1.45(b,2H),1.67(c,3H),3.2-3.7(d), 5.3-5.8(e,2H)	83Kre
218	C ₅ H ₁₁ NO	CDCl ₃	1.52(a,9H),6.49(b),6.56(c)	89War
219	C ₅ H ₁₁ NO	CDCl ₃	8.03(a),3.26(b,4H),1.2(c,6H)	91Nev
220	C ₅ H ₁₁ NOS	CDCl ₃ 37°C	0.97(a,3H),1.61(b,2H),2.09(c,3H),2.67(d,2H), 7.16(e)	72Kis
221	C ₅ H ₁₁ NO ₂	CDCl ₃	4.42(a),1.97(b,4H),1.03(c,6H)	92Asa
222	C ₅ H ₁₁ NO ₃ S	CDCl ₃	1.0(a,3H),1.5(b,3H),2.5-3.0(c,2H),4.2(d), 6.4(e,2H)	85Ben
223	C ₅ H ₁₁ NO ₄	CDCl ₃	2.3(a,2H),3.4(b,6H),4.55(c,3H)	86Öhr
224	C ₅ H ₁₁ N ₃ OS	CDCl ₃	1.36(a,6H),3.46(b,3H),4.67(c),8.26(d)	85Iso
225	C ₅ H ₁₂ ClN	CDCl ₃	0.9(a,3H),1.12-1.75(b,4H),2.83(c,2H),2.88(d,3H)	88Gui

No.	Gross formula	Solvent	δ [ppm]	Ref.
226	C ₅ H ₁₂ N ₂ O	CDCl ₃	0.92(a,6H),1.75(b,3H),2.97(c),4.1–4.7(d), 8.2–8.8(e)	95Wu
227	C ₅ H ₁₂ N ₄ O ₂	CDCl ₃	1.78(a),2.94(b,3H),3.26(c,3H),3.97(d,2H), 4.02(e,2H),6.34(f)	88Smi
228	C ₅ H ₁₂ O ₂ S	CDCl ₃	4.45(a),3.36(b,6H),2.64(c,2H),2.16(d,3H)	79McC
229	C ₅ H ₁₂ O ₃	CD ₃ COCD ₃	1.15(a,3H),1.73(b,2H),3.4(c,2H),3.75(d,2H), 3.95(e,3H)	82Bon
230	C ₅ H ₁₂ O ₃	CDCl ₃	2.0(a),3.09(b,2H),3.35(c,3H),3.53(d,2H), 3.77(e,4H)	98Ale
231	C ₅ H ₁₃ NS	CDCl ₃	1.1(a),1.3(b,6H),2.5(c,3H),2.6(d,2H)	75D'Am
232	C ₅ H ₁₄ ClNO ₂	D ₂ O	1.17(a,3H),2.94(b,3H),3.13(c,2H),3.64(d,2H), 5.38(e)	78Bow
233	C ₅ H ₁₄ ClNS	CD ₃ NO ₂	2.83(a,6H),2.2(b,3H),3.0–3.7(c,4H)	89Kim
234	C ₅ H ₁₄ Cl ₂ N ₂ O ₂	D ₂ O	3.12(a),3.36(b,2H),2.68(c,2H),1.88–2.19(d,2H)	84Alt
235	C ₆ H ₂ Cl ₄ O ₄ S ₂	CDCl ₃	8.65(a),8.4(b)	88Puy
236	C ₆ H ₃ BrF ₈	CDCl ₃	4.11(a,2H),6.0(b)	95Pet
237	C ₆ H ₄ Cl ₂ F ₆ O	CCl ₄	2.83(a),2.9(b,2H),5.97(c)	77Sey
238	C ₆ H ₅ F ₃ O ₂	THF-d ₈	2.57(a,4H),9.77(b)	85Bla2
239	C ₆ H ₅ F ₄ NO ₂	CCl ₄	4.54(a,2H),1.43(b,3H)	86Kre1
240	C ₆ H ₅ F ₇ O ₃	CCl ₄	4.21(a,2H),3.84(b,3H)	84Kre
241	C ₆ H ₆ ClF ₃ O ₂	CDCl ₃	6.2(a),4.4(b,2H),1.4(c,3H)	90The
242	C ₆ H ₆ Cl ₂	CCl ₄	5.67(a,2H),2.94(b,4H)	80Wis
243	C ₆ H ₆ Cl ₂ F ₂ O	CDCl ₃	3.24(a,2H),3.81(b,3H),6.27(c)	86Pas
244	C ₆ H ₆ Cl ₃ NO	CDCl ₃	2.06(a,3H),3.18&3.3(b,2H),9.2(c)	85Mar
245	C ₆ H ₆ FN ₃ O ₂	CDCl ₃ 25°C	3.2&5.6(a,4H),6.42(b),6.82(c)	93Tia
246	C ₆ H ₆ F ₄ O ₃	–	5.1(a),4.3(b,2H),1.3(c,3H)	90The
247	C ₆ H ₆ F ₆ O	CCl ₄	1.49(a,3H),3.79(b),5.02(c),6.22(d)	91Nis
248	C ₆ H ₆ F ₆ OS ₂	CDCl ₃	1.4(a,3H),4.25(b,2H),7.47(c)	98Kol
249	C ₆ H ₆ F ₆ O ₂	–	1.67(a,3H),4.2(b,2H),5.78(c)	85Cha1
250	C ₆ H ₆ F ₆ O ₂	–	2.77(a,2H),3.32(b,3H),5.08(c)	85Caa1
251	C ₆ H ₆ F ₂ O ₂	–	1.35(a,3H),4.38(b,2H),5.23(c)	93Muz1
252	C ₆ H ₆ O ₂	CCl ₄	2.9(a),4.63(b,2H),5.2–5.43(c,2H),5.91(d)	86Pad
253	C ₆ H ₇ ClO	CDCl ₃	6.28(a),1.8–2.9(b,6H)	81Kow