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Magnetische Kernresonanz

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Arbeitsgruppe: Stark korrelierte Elektronen und Spins

Magnetische Kernresonanz

Was wird gemacht?

Untersuchung verschiedener Proben mittels magnetischer Kernresonanzspektroskopie (NMR).

Aufgabe

1. Kalibrierung des magnetischen Feldes durch Messung des NMR-Spektrums einer Glycerinprobe
2. Analoge Ermittlung des g-Faktors und des gyromagnetischen Verhältnis γ folgender Proben:
 - a. Teflon
 - b. Kupfersulfat
 - c. Polystyrol
3. Bestimmung der Art des Kernmoments, welches im Experiment angeregt wurde

Hintergrund

- ✓ Spin und magnetisches Moment
- ✓ g-Faktor und gyromagnetischen Verhältnis γ
- ✓ Magnetische Energie; Energie eines Protons/Elektrons im äußeren Magnetfeld
- ✓ Kernmagneton und Bohrsches Magneton
- ✓ Larmorpräzession und –frequenz
- ✓ Magnetische Kernresonanz: Prinzip und Realisation

Empfohlene Literatur

Versuchsanleitung

Gyromagnetic Ratio

In physics, the **gyromagnetic ratio** (also sometimes known as the **magnetogyric ratio** in other disciplines) of a particle or system is the ratio of its magnetic dipole moment to its angular momentum, and it is often denoted by the symbol γ , gamma. Its SI units are radian per second per tesla ($\text{s}^{-1}\text{T}^{-1}$) or, equivalently, coulomb per kilogram (C/kg).

Gyromagnetic Ratio and Larmor Precession

Any free system with a constant gyromagnetic ratio, such as a rigid system of charges, a nucleus, or an electron, when placed in an external magnetic field B (measured in teslas) that is not aligned with its magnetic moment, will precess at a frequency f (measured in hertz), that is proportional to the external field:

$$f = \frac{\gamma}{2\pi} B$$

For this reason, values of $\gamma/(2\pi)$, in units of hertz per tesla (Hz/T), are often quoted instead of γ .

This relationship also explains an apparent contradiction between the two equivalent terms, **gyromagnetic ratio** versus **magnetogyric ratio**: whereas it is a ratio of a magnetic property (i.e. dipole moment) to a *gyric* (rotational, from Greek: $\gamma\acute{\upsilon}\rho\omicron\varsigma$, "turn") property (i.e. angular momentum), it is also, *at the same time*, a ratio between the angular precession frequency (another *gyric* property) $\omega = 2\pi f$ and the magnetic field.

Nuclear Magneton

The **nuclear magneton** (symbol μ_{N}), is a physical constant of magnetic moment, defined by:

$$\mu_{\text{N}} = \frac{e\hbar}{2m_{\text{p}}}$$

where:

e is the elementary charge,
 \hbar is the reduced Planck's constant,
 m_{p} is the proton rest mass

In the SI system of units its value is approximately:

$$\mu_{\text{N}} = 5.050\,783\,24(13) \times 10^{-27} \text{ J T}^{-1}$$

Bohr Magnetron

In atomic physics, the **Bohr magneton** (symbol μ_B) is named after the physicist Niels Bohr. It is a physical constant of magnetic moment, defined in SI units by

$$\mu_B = \frac{e\hbar}{2m_e}$$

and in Gaussian centimeter-gram-second units by

$$\mu_B = \frac{e\hbar}{2m_e c}$$

where

e is the elementary charge,
 \hbar is the reduced Planck's constant,
 m_e is the electron rest mass
 c is the speed of light.

In the SI system of units its value is

$$\mu_B = 9.274\,009\,49(80) \times 10^{-24} \text{ J}\cdot\text{T}^{-1}.$$

In the eV system of units its value is

$$\mu_B = 5.7883 \times 10^{-5} \text{ eV}\cdot\text{T}^{-1}.$$

In the CGS system of units its value is

$$\mu_B = 0.927 \times 10^{-20} \text{ Erg}\cdot\text{Oe}^{-1} \text{ [1]}$$

The Bohr magneton is the natural unit for expressing the electron magnetic dipole moment in the hydrogen atom. It was first calculated by Romanian physicist Stefan Procopiu around 1910 and in some Romanian literature is called the Bohr-Procopiu Magnetron. An electron has an intrinsic magnetic dipole moment of approximately one Bohr magneton.

Larmor Precession

In physics, **Larmor precession** (named after Joseph Larmor) refers to the precession of the magnetic moments of electrons, atomic nuclei, and atoms about an external magnetic field. The magnetic field exerts a torque on the magnetic moment,

$$\vec{\Gamma} = \vec{\mu} \times \vec{B} = \gamma \vec{J} \times \vec{B}$$

where $\vec{\Gamma}$ is the torque, \vec{J} is the angular momentum vector, \vec{B} is the external magnetic field, \times is the cross product, and γ is the gyromagnetic ratio which gives the proportionality constant between the magnetic moment and the angular momentum. The angular momentum vector \vec{J} precesses about the external field axis with an angular frequency known as the **Larmor frequency**,

$$\omega = \gamma B$$

where ω is the angular frequency and B is the magnitude of the magnetic field.

Larmor precession is important in nuclear magnetic resonance.

Magnetic energy

There is no fundamental difference between magnetic energy and electric energy: the two phenomena are related by Maxwell's equations. The potential energy of a magnet of magnetic moment \mathbf{m} in a magnetic field \mathbf{B} is defined as the work of magnetic force (actually of magnetic torque) on re-alignment of the vector of the magnetic dipole moment, and is equal:

$$E_{p,m} = -\mathbf{m} \cdot \mathbf{B}$$

while the energy stored in a inductor (of inductance L) when current I is passing via it is

$$E_{p,m} = \frac{1}{2}LI^2$$

This second expression forms the basis for superconducting magnetic energy storage.

Nuclear Properties of Spin 1/2 Nuclei

Table 1.1 NMR Properties of the Spin-1/2 Nuclei^a

Isotope ^b	Natural abundance ^c C/%	Magnetic moment ^d μ/μ_N	Magnetogyric ratio ^e $\gamma/10^7 \text{ rad T}^{-1} \text{ s}^{-1}$	NMR frequency ^e ν/MHz	Standard	Relative receptivity ^f	
						D^P	D^C
¹ H	99.985	4.83724	26.7519	100.000 000	Me ₄ Si	1.000	5.67 × 10 ³
² H ^g	-	5.1596	28.535	(106.664)	Me ₄ Si-t	-	-
³ He	1.3 × 10 ⁻⁴	-3.6851	-20.380	(76.182)	-	5.75 × 10 ⁻⁷	3.26 × 10 ⁻³
¹³ C	1.108	1.2166	6.7283	25.145 004	Me ₄ Si	1.76 × 10 ⁻³	1.00
¹⁵ N	0.37	-0.4903	-2.712	10.136 783	MeNO ₂ or [NO ₃] ⁻	3.85 × 10 ⁻⁶	2.19 × 10 ⁻²
¹⁹ F	100	4.5532	25.181	94.094 003 ⁱ	CCl ₃ F	0.834	4.73 × 10 ³
²⁹ Si	4.70	-0.96174	-5.3188	19.867 184	Me ₄ Si	3.69 × 10 ⁻⁴	2.10
³¹ P	100	1.9602	10.841	40.480 737	85% H ₃ PO ₄	0.0665	3.77 × 10 ²
⁵⁷ Fe	2.19	0.1566	0.8661	(3.238)	Fe(CO) ₅	7.43 × 10 ⁻⁷	4.22 × 10 ⁻³
⁷⁷ Se	7.58	0.925	5.12	19.071 523	Me ₂ Se	5.30 × 10 ⁻⁴	3.01
⁸⁹ Y	100	-0.23786	-1.3155	(4.917)	Y(NO ₃) ₃ aq.	1.19 × 10 ⁻⁴	0.675
¹⁰³ Rh	100	-0.153	-0.846	3.172 310	mer-[RhCl ₃ (SMe ₂) ₃]	3.16 × 10 ⁻⁵	0.179
(¹⁰⁷ Ag)	51.82	-0.1966	-1.087	4.047 897	Ag ⁺ aq.	3.43 × 10 ⁻⁵	0.197
¹⁰⁹ Ag	48.18	-0.2260	-1.250	4.653 623		4.92 × 10 ⁻⁵	0.279
(¹¹¹ Cd)	12.75	-1.0293	-5.6926	21.215 478	CdMe ₂	1.23 × 10 ⁻³	6.97
¹¹³ Cd ^h	12.26	-1.0768	-5.9550	22.193 173		1.35 × 10 ⁻³	7.67
(¹¹⁵ Sn)	0.35	-1.590	-8.792	(32.86)	Me ₄ Sn	1.24 × 10 ⁻⁴	0.705
(¹¹⁷ Sn)	7.61	-1.732	-9.578	35.632 295		3.49 × 10 ⁻³	19.8
¹¹⁹ Sn	8.58	-1.8119	-10.021	37.290 662		4.51 × 10 ⁻³	25.6
(¹²³ Te ^h)	0.87	-1.275	-7.049	(26.35)	Me ₂ Te	1.59 × 10 ⁻⁴	0.903
¹²⁵ Te	6.99	-1.537	-8.498	31.549 802		2.24 × 10 ⁻³	12.7
¹²⁹ Xe	26.44	-1.345	-7.441	(27.81)	XeOF ₄	5.69 × 10 ⁻³	32.3
¹⁶⁹ Tm	100	-0.400	-2.21	(8.27)	-	5.66 × 10 ⁻⁴	3.21
¹⁷¹ Yb	14.31	0.8520	4.712	(17.61)	-	7.82 × 10 ⁻⁴	4.44
¹⁸³ W	14.40	0.2025	1.120	4.161 733	WF ₆	1.06 × 10 ⁻⁵	5.99 × 10 ⁻²
¹⁸⁷ Os	1.64	0.111	0.616	2.282 343	OsO ₄	2.00 × 10 ⁻⁷	1.14 × 10 ⁻³
¹⁹⁵ Pt	33.8	1.043	5.768	21.414 376	[Pt(CN) ₆] ²⁻	3.39 × 10 ⁻³	19.2
¹⁹⁹ Hg	16.84	0.87072	4.8154	17.910 841	Me ₂ Hg	9.82 × 10 ⁻⁴	5.57
(²⁰³ Tl)	29.50	2.7912	15.436	(57.70)	TlNO ₃ aq.	0.0567	3.22 × 10 ²
²⁰⁵ Tl	70.50	2.8187	15.589	57.633 833		0.140	7.91 × 10 ²
²⁰⁷ Pb	22.6	1.002	5.540	20.920 597	Me ₄ Pb	2.01 × 10 ⁻³	11.4

D^P is sensitivity relative to ¹H.

D^C is sensitivity relative to ¹³C.

Although not in this table, often tables include Absolute Sensitivity and Relative Sensitivity. Relative Sensitivity is the sensitivity of the nucleus relative to either ¹H or ¹³C, without including the natural abundance. Absolute Sensitivity is the product of the Relative Sensitivity and the natural abundance.

In the table above, both D^P and D^C are Absolute Sensitivity (so the natural abundance is included in the sensitivity).

Measuring of the applied magnetic field:

- ✓ NMR (permanent magnet system). In order to measure a magnetic field of a constant magnet you can use the sensor (induction coil with the integrator) used for Zeeman-Effect. To compare with the values obtained from the frequency measurements
- ✓ ESR (Geometrie der Helmholtzspule). To make the calculation of the magnetic field of the Helmholtz coil on the basis of its geometrical parameters. To explain, why this configuration for making a magnetic field was chosen?

To measure the frequency-field dependence for DPPH sample (frequency range 28.8-38.5 MHz; current range for Helmholtz coil 0.717-0.954 A).

Table of Other NMR Active Nuclei

Table 1.2 The Spin Properties of Quadrupolar Nuclei^a

Isotope ^b	Spin ^c	Natural abundance ^c C/%	Magnetic moment ^d μ/μ _N	Magnetogyric ratio ^e γ/10 ⁷ rad T ⁻¹ s ⁻¹	Quadrupole moment ^f 10 ⁻²⁸ Q/m ²	NMR frequency ^g ν/MHz	Linewidth factor ^h 10 ³⁶ C/m ⁴	Relative receptivity ⁱ	
								D ^F	D ^C
² He	1	0.015	1.2126	4.1066	2.8 × 10 ⁻³	15.351	3.9 × 10 ⁻³	1.45 × 10 ⁻⁶	8.21 × 10 ⁻³
⁶ Li	1	7.42	1.1625	3.9371	-8 × 10 ⁻¹	14.717	3.2 × 10 ⁻⁶	6.31 × 10 ⁻¹	3.58
⁷ Li	3/2	92.58	4.20394	10.3975	-4 × 10 ⁻²	38.866	2.1 × 10 ⁻³	0.272	1.54 × 10 ³
⁹ Be	3/2	100	-1.52008	-3.7598	5 × 10 ⁻²	14.054	3.3 × 10 ⁻³	1.39 × 10 ⁻²	78.7
¹⁰ B	3	19.58	2.0792	2.8746	8.5 × 10 ⁻²	10.746	1.4 × 10 ⁻³	3.93 × 10 ⁻³	22.3
¹¹ B	3/2	80.42	3.4708	8.5843	4.1 × 10 ⁻²	32.089	2.2 × 10 ⁻³	0.133	7.52 × 10 ²
¹⁴ N	1	99.63	0.57099	1.9338	1 × 10 ⁻²	7.228	5.0 × 10 ⁻¹	1.00 × 10 ⁻³	5.69
¹⁶ O	5/2	0.057	-2.2407	-3.6279	-2.6 × 10 ⁻²	13.561	2.2 × 10 ⁻¹	1.08 × 10 ⁻³	6.11 × 10 ⁻²
²¹ Ne	3/2	0.257	-0.85433	-2.1150	9 × 10 ⁻²	7.899	1.1 × 10 ⁻²	6.33 × 10 ⁻⁶	3.59 × 10 ⁻²
²³ Na	3/2	100	2.86265	7.08013	0.10	26.466	1.3 × 10 ⁻²	9.27 × 10 ⁻²	5.26 × 10 ²
²⁵ Mg	5/2	10.13	-1.012	-1.639	0.22	6.126	1.5 × 10 ⁻²	2.72 × 10 ⁻⁴	1.54
²⁷ Mg	3/2	5/2	4.3084	6.9760	0.15	26.077	7.2 × 10 ⁻³	0.207	1.17 × 10 ³
²⁷ Al	5/2	100	4.3084	6.9760	0.15	26.077	7.2 × 10 ⁻³	0.207	1.17 × 10 ³
³¹ P	3/2	0.76	0.8908	2.055	-5.5 × 10 ⁻²	7.681	4.0 × 10 ⁻³	1.72 × 10 ⁻⁵	9.77 × 10 ⁻¹
³³ P	3/2	75.53	1.0610	2.6240	-0.10	9.509	1.3 × 10 ⁻²	3.56 × 10 ⁻³	20.2
³⁵ Cl	3/2	24.47	0.88313	2.1842	-7.9 × 10 ⁻²	8.165	8.3 × 10 ⁻³	4.66 × 10 ⁻³	3.78
³⁷ Cl	3/2	75.53	1.0610	2.6240	-0.10	9.509	1.3 × 10 ⁻²	3.56 × 10 ⁻³	20.2
³⁹ K	3/2	93.1	0.50553	1.2498	4.9 × 10 ⁻²	4.672	3.2 × 10 ⁻³	4.75 × 10 ⁻¹	2.69
⁴¹ K	3/2	6.88	0.27740	0.68608	6.0 × 10 ⁻²	2.565	4.8 × 10 ⁻³	5.80 × 10 ⁻⁶	3.29 × 10 ⁻¹
⁴⁰ Ca	7/2	0.145	-1.4936	-1.8025	0.2	6.738	5.4 × 10 ⁻³	8.67 × 10 ⁻⁶	4.92 × 10 ⁻²
⁴² Ca	7/2	100	5.3927	6.5081	-0.22	24.328	6.6 × 10 ⁻³	0.302	1.72 × 10 ³
⁴³ Ca	7/2	100	5.3927	6.5081	-0.22	24.328	6.6 × 10 ⁻³	0.302	1.72 × 10 ³
⁴⁷ Ti	5/2	7.23	-0.93292	-1.5105	0.29	5.646	2.7 × 10 ⁻²	1.53 × 10 ⁻¹	0.867
⁴⁹ Ti	7/2	5.51	-1.25198	-1.51093	0.24	5.648	7.8 × 10 ⁻³	2.08 × 10 ⁻¹	1.18
⁵¹ V	7/2	0.24	3.6152	2.6717	±6 × 10 ⁻²	9.987	1.4 × 10 ⁻¹	1.34 × 10 ⁻¹	0.759
⁵¹ V	7/2	99.76	3.8379	7.0455	-5 × 10 ⁻²	26.336	3.4 × 10 ⁻¹	0.383	2.17 × 10 ³
⁵³ Cr	3/2	9.55	-0.6113	-1.512	-0.15	5.621	1.2 × 10 ⁻³	8.62 × 10 ⁻⁵	0.439
⁵⁵ Mn	5/2	100	4.081	6.608	0.4	24.70	5.1 × 10 ⁻²	0.176	9.97 × 10 ²
⁵⁹ Co	7/2	100	5.234	6.317	0.38	23.61	2.0 × 10 ⁻²	0.277	1.57 × 10 ³
⁶⁰ Ni	3/2	1.19	-0.9680	-2.394	0.16	8.949	3.4 × 10 ⁻²	4.06 × 10 ⁻³	0.231
⁶⁴ Cu	3/2	69.09	2.8696	7.0974	-0.211	26.530	5.94 × 10 ⁻²	6.45 × 10 ⁻²	3.66 × 10 ²
⁶⁵ Cu	3/2	30.91	3.0741	7.6031	-0.195	28.421	5.07 × 10 ⁻²	3.55 × 10 ⁻²	2.01 × 10 ²
⁶⁶ Cu	3/2	4.11	1.0356	1.6768	0.16	6.2679	8.2 × 10 ⁻³	1.18 × 10 ⁻¹	0.670
⁶⁷ Zn	5/2	60.4	2.6007	6.4323	0.19	24.044	4.9 × 10 ⁻²	4.19 × 10 ⁻²	2.38 × 10 ²
⁶⁹ Ga	3/2	39.6	3.2046	8.1731	0.12	30.551	1.9 × 10 ⁻²	5.65 × 10 ⁻²	3.20 × 10 ²
⁷¹ Ga	3/2	39.6	3.2046	8.1731	0.12	30.551	1.9 × 10 ⁻²	5.65 × 10 ⁻²	3.20 × 10 ²
⁷³ Ge	9/2	7.76	-0.97197	-0.93574	-0.18	3.498	2.4 × 10 ⁻³	1.10 × 10 ⁻¹	0.622
⁷⁵ As	3/2	100	1.858	4.595	0.29	17.18	0.11	2.53 × 10 ⁻²	1.44 × 10 ²
⁷⁹ Br	3/2	50.54	2.7182	6.7228	0.37	25.150	0.18	4.01 × 10 ⁻²	2.28 × 10 ²
⁸¹ Br	3/2	49.46	2.9300	7.2468	0.31	27.089	0.15	4.92 × 10 ⁻²	2.79 × 10 ²
⁸³ Kr	9/2	11.55	-1.073	-1.033	0.26	3.860	5.0 × 10 ⁻³	2.19 × 10 ⁻¹	1.24
⁸⁵ Rb	5/2	72.15	1.6002	2.5909	0.26	9.685	2.2 × 10 ⁻²	7.65 × 10 ⁻³	43.4
⁸⁷ Rb	3/2	27.85	3.5502	8.7807	0.13	32.823	2.3 × 10 ⁻²	4.92 × 10 ⁻²	2.79 × 10 ²
⁸⁹ Sr	9/2	7.02	-1.208	-1.163	0.3	4.349	6.7 × 10 ⁻³	1.91 × 10 ⁻¹	1.08
⁹¹ Zr	5/2	11.23	-1.5415	-2.4939	-0.21	9.3298	1.4 × 10 ⁻²	1.06 × 10 ⁻³	6.04
⁹³ Nb	9/2	100	6.618	6.564	-0.22	24.54	3.6 × 10 ⁻³	0.487	2.77 × 10 ³
⁹⁵ Mo	5/2	15.72	1.081	1.750	-0.022	6.542	4.6 × 10 ⁻³	5.14 × 10 ⁻⁴	2.92
⁹⁷ Mo	5/2	9.46	-1.104	-1.787	0.255	6.679	0.39	3.29 × 10 ⁻⁴	1.87
⁹⁹ Tc	9/2	-	6.281	6.046	0.3	22.60	6.7 × 10 ⁻³	-	-
⁹⁹ Tc	9/2	-	6.281	6.046	0.3	22.60	6.7 × 10 ⁻³	-	-
¹⁰¹ Ru	5/2	12.72	-0.7622 ^m	-1.234 ^m	7.6 × 10 ⁻²	4.614 ^m	1.8 × 10 ⁻³	1.46 × 10 ⁻¹	0.327
¹⁰¹ Ru	5/2	17.07	-0.8544 ^m	-1.383 ^m	0.44	5.171 ^m	6.2 × 10 ⁻²	2.73 × 10 ⁻¹	1.56
¹⁰² Ru	5/2	17.07	-0.8544 ^m	-1.383 ^m	0.44	5.171 ^m	6.2 × 10 ⁻²	2.73 × 10 ⁻¹	1.56
¹⁰³ Ru	5/2	17.07	-0.8544 ^m	-1.383 ^m	0.44	5.171 ^m	6.2 × 10 ⁻²	2.73 × 10 ⁻¹	1.56
¹⁰⁵ Pd	5/2	22.23	-0.760	-1.23	0.8	4.60	0.20	2.52 × 10 ⁻¹	1.43
¹¹³ In	9/2	4.28	6.1058	5.8782	0.82	21.973	5.0 × 10 ⁻²	1.50 × 10 ⁻²	85.0
¹¹⁵ In	9/2	95.72	6.1190	5.8908	0.83	22.020	5.1 × 10 ⁻²	0.337	1.91 × 10 ³
¹²¹ Sb	5/2	57.25	3.9747	6.4355	-0.28	24.056	2.5 × 10 ⁻²	9.30 × 10 ⁻²	5.27 × 10 ²
¹²³ Sb	7/2	42.75	2.8876	3.4848	-0.36	13.026	1.8 × 10 ⁻²	1.98 × 10 ⁻²	1.13 × 10 ²
¹²⁵ Sb	7/2	42.75	2.8876	3.4848	-0.36	13.026	1.8 × 10 ⁻²	1.98 × 10 ⁻²	1.13 × 10 ²
¹²⁷ I	5/2	100	3.3238	5.3817	-0.79	20.117	0.20	9.20 × 10 ⁻²	5.39 × 10 ²
¹²⁹ Xe	3/2	21.18	0.8918	2.206	-0.12	8.245	1.9 × 10 ⁻²	5.94 × 10 ⁻¹	3.37
¹³³ Cs	7/2	100	2.9231	3.5277	-3 × 10 ⁻³	13.187	1.2 × 10 ⁻⁶	4.82 × 10 ⁻²	2.73 × 10 ²
¹³⁵ Ba	3/2	6.59	1.080	2.671	0.18	9.984	4.3 × 10 ⁻²	3.28 × 10 ⁻¹	1.86
¹³⁷ Ba	3/2	11.32	1.208	2.988	0.28	11.17	0.10	7.89 × 10 ⁻¹	4.47
¹³⁹ Ba	7/2	99.911	3.150	3.801	0.22	14.210	6.6 × 10 ⁻³	6.02 × 10 ⁻²	3.42 × 10 ²
¹⁷⁷ Hf	7/2	18.50	0.8960	1.081	4.5	4.042	2.8	2.57 × 10 ⁻¹	1.46
¹⁷⁹ Hf	9/2	13.75	-0.705	-0.679	5.1	2.54	1.9	7.42 × 10 ⁻¹	0.421
¹⁸¹ Ta	7/2	99.988	2.66	3.22	3	12.0	1.2	3.65 × 10 ⁻²	2.07 × 10 ²
¹⁸³ Re	5/2	37.07	3.753	6.077	2.3	22.72	1.7	5.13 × 10 ⁻²	2.91 × 10 ²
¹⁸⁷ Re	5/2	62.93	3.791	6.138	2.2	22.94	1.5	8.81 × 10 ⁻²	5.00 × 10 ²
¹⁸⁹ Os	3/2	16.1	0.8475	2.096	0.8	7.836	0.85	3.87 × 10 ⁻¹	2.20
¹⁹¹ Ir	3/2	37.3	0.1877	0.4643	1.1	1.735	1.6	9.77 × 10 ⁻⁶	5.54 × 10 ⁻²
¹⁹³ Ir	3/2	62.7	0.2044	0.5054	1.0	1.889	1.3	2.11 × 10 ⁻⁵	0.120
¹⁹⁷ Au	3/2	100	0.15701	0.46254	0.59	1.729	0.46	2.58 × 10 ⁻⁵	0.147
²⁰¹ Hg	3/2	13.22	-0.71871	-1.7776	0.44	6.645	0.26	1.94 × 10 ⁻¹	1.10
²⁰³ Bi	9/2	100	4.511	4.342	-0.38	16.23	1.1 × 10 ⁻²	0.141	8.01 × 10 ³

NMR Periodic Table

Prepared at the Laboratory for Magnetic Resonance
and Molecular Spectroscopy, University of Groningen

$$\left\{ \frac{e}{m_N}; g_N; \gamma_N \right\}$$

$$\text{Nuclear magneton: } \mu_N = \frac{e\hbar}{2m_p} = 5.05078343 \cdot 10^{-27} \text{ JT}^{-1}$$

Hydrogen

Note: Resonance frequencies are quoted relative to a resonance frequency of exactly 100 (2.3488 T), 200 (4.6975 T), and 300 (7.0463 T) MHz for ^1H

Isotope: ^1H

Spin:	$S=1/2$
Natural abundance:	99.985%
Gyromagnetic ratio ($\text{rad}\cdot\text{s}^{-1}\cdot\text{T}^{-1}$):	$\gamma=26.7520 \times 10^7$
Landé g-factor $g = \frac{\gamma\hbar}{\mu_N} = \frac{\gamma 2m_p}{e}$:	$g=5.58564$
Relative receptivity:	1.00
Magnetic moment μ/μ_N :	4.83724
Quadrupole moment $Q/m(2)$:	0
NMR Resonance frequency	100, 200 and 300 MHz
$\omega = 2\pi f = \gamma B \Rightarrow \frac{f}{B} = \frac{\gamma}{2\pi}$ (MHz/T):	42.5771

Isotope: ^2H

Spin:	$S=1$
Natural abundance:	0.015%
Gyromagnetic ratio ($\text{rad}\cdot\text{s}^{-1}\cdot\text{T}^{-1}$):	$\gamma=4.1066 \times 10^7$
Relative receptivity:	0.00000145
Magnetic Moment μ/μ_N :	1.2126
Quadrupole moment $Q/m(2)$:	$0.0028 \times 10(28)$
NMR Resonance frequency	15.351, 30.701, 46.051 MHz

Isotope: ^3H

Spin:	$S=1/2$
Natural abundance:	---
Gyromagnetic ratio ($\text{rad}\cdot\text{s}^{-1}\cdot\text{T}^{-1}$):	$\gamma=28.535 \times 10^7$
Relative receptivity:	1.21
Magnetic Moment μ/μ_N :	5.1596
Quadrupole moment $Q/m(2)$:	0
NMR Resonance frequency	106.663, 213.327, 319.990 MHz

NMR Periodic Table

Prepared by the Laboratory for Magnetic Resonance
and Molecular Crystals, University of Illinois

Fluorine

Note: Resonance frequencies are quoted relative to a resonance frequency of exactly 100 MHz for ^1H .

Isotope: ^{19}F

Spin:	$S=1/2$
Natural abundance:	100%
Gyromagnetic ratio ($\text{rad}\cdot\text{s}^{-1}\cdot\text{T}^{-1}$):	$\gamma=25.181 \times 10^7$
Landé g-factor $g = \frac{\hbar}{\mu_N} = \frac{\gamma 2m_p}{e}$:	$g=5.25505$
Relative receptivity:	0.834
Magnetic moment μ/μ_N :	4.5532
Quadrupole moment $Q/\text{m}(2)$:	0
NMR Resonance frequency:	94.077 MHz
$\omega = 2\pi f = \gamma B \Rightarrow \frac{f}{B} = \frac{\gamma}{2\pi}$ (MHz/T):	40.0768

Nuclear Magnetic Resonance Spectroscopy

Background

Over the past fifty years nuclear magnetic resonance spectroscopy, commonly referred to as NMR, has become the preeminent technique for determining the structure of organic compounds. Of all the spectroscopic methods, it is the only one for which a complete analysis and interpretation of the entire spectrum is normally expected. Although larger amounts of sample are needed than for mass spectroscopy, nmr is non-destructive, and with modern instruments good data may be obtained from samples weighing less than a milligram. **To be successful in using NMR as an analytical tool, it is necessary to understand the physical principles on which the methods are based.**

The nuclei of many elemental isotopes have a characteristic spin (I). Some nuclei have integral spins (e.g. $I = 1, 2, 3 \dots$), some have fractional spins (e.g. $I = 1/2, 3/2, 5/2 \dots$), and a few have no spin, $I = 0$ (e.g. ^{12}C , ^{16}O , ^{32}S ,). Isotopes of particular interest and use to organic chemists are ^1H , ^{13}C , ^{19}F and ^{31}P , all of which have $I = 1/2$. Since the analysis of this spin state is fairly straightforward, our discussion of nmr will be limited to these and other $I = 1/2$ nuclei.

Spin Properties of Nuclei

Nuclear spin may be related to the nucleon composition of a nucleus in the following manner:

◆ Odd mass nuclei (i.e. those having an odd number of nucleons) have fractional spins. Examples are $I = 1/2$ (^1H , ^{13}C , ^{19}F), $I = 3/2$ (^{11}B) & $I = 5/2$ (^{17}O).

◆ Even mass nuclei composed of odd numbers of protons and neutrons have integral spins. Examples are $I = 1$ (^2H , ^{14}N).

◆ Even mass nuclei composed of even numbers of protons and neutrons have zero spin ($I = 0$). Examples are ^{12}C , and ^{16}O .

Spin $1/2$ nuclei have a spherical charge distribution, and their NMR behavior is the easiest to understand. Other spin nuclei have nonspherical charge distributions and may be analyzed as prolate or oblate spinning bodies. All nuclei with non-zero spins have magnetic moments (μ), but the nonspherical nuclei also have an electric quadrupole moment (eQ). Some characteristic properties of selected nuclei are given in the following table.

Isotope	Natural % Abundance	Spin (I)	Magnetic Moment (μ)	Magnetogyric Ratio (γ) *
^1H	99.9844	1/2	2.7927	26.753
^2H	0.0156	1	0.8574	4,107
^{11}B	81.17	3/2	2.6880	--
^{13}C	1.108	1/2	0.7022	6,728
^{17}O	0.037	5/2	-1.8930	-3,628
^{19}F	100.0	1/2	2.6273	25,179
^{29}Si	4.700	1/2	-0.5555	-5,319
^{31}P	100.0	1/2	1.1305	10,840

* γ has units of $10^7 \text{ rad T}^{-1} \text{ sec}^{-1}$

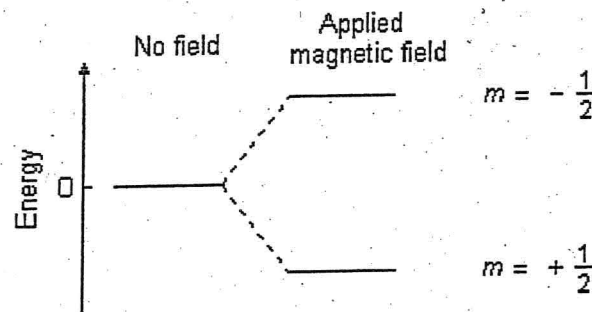
Nuclear spin and the splitting of energy levels in a magnetic field

Subatomic particles (electrons, protons and neutrons) can be imagined as spinning on their axes. In many atoms (such as ^{12}C) these spins are paired against each other, such that the nucleus of the atom has no overall spin. However, in some atoms (such as ^1H and ^{13}C) the nucleus does possess an overall spin. The rules for determining the net spin of a nucleus are as follows;

1. If the number of neutrons **and** the number of protons are both even, then the nucleus has **NO** spin.
2. If the number of neutrons **plus** the number of protons is odd, then the nucleus has a half-integer spin (i.e. $1/2, 3/2, 5/2$)
3. If the number of neutrons **and** the number of protons are both odd, then the nucleus has an integer spin (i.e. $1, 2, 3$)

The overall spin, I , is important. Quantum mechanics tells us that a nucleus of spin I will have $2I + 1$ possible orientations. A nucleus with spin $1/2$ will have 2 possible orientations. In the absence of an external magnetic field, these orientations are of equal energy. If a magnetic field is applied, then the energy levels split. Each level is given a *magnetic quantum number*, m .

Energy levels for a nucleus with spin quantum number $1/2$



When the nucleus is in a magnetic field, the initial populations of the energy levels are determined by thermodynamics, as described by the Boltzmann distribution. This is very important, and it means that **the lower energy level will contain slightly more nuclei than the higher level**. It is possible to excite these nuclei into the higher level with electromagnetic radiation. The frequency of radiation needed is determined by the difference in energy between the energy levels.

Calculating transition energy

The nucleus has a positive charge and is spinning. This generates a small magnetic field. The nucleus therefore possesses a magnetic moment, μ , which is proportional to its spin, I .

$$\mu = \frac{\gamma I h}{2\pi}$$

The constant, γ , is called the *magnetogyric ratio* and is a fundamental nuclear constant which has a different value for every nucleus. h is Planck's constant.

$\gamma = \text{gyromagnetic ratio}$

The energy of a particular energy level is given by;

$$\gamma = \frac{\mu}{I} \text{ (ang. momentum)}$$

$$f = \frac{\gamma}{2\pi} B$$

$$E = - \frac{\gamma \hbar}{2 \pi} m B$$

Where B is the strength of the magnetic field **at the nucleus**.

The difference in energy between levels (the transition energy) can be found from

$$\Delta E = \frac{\gamma \hbar B}{2 \pi} \quad \checkmark$$

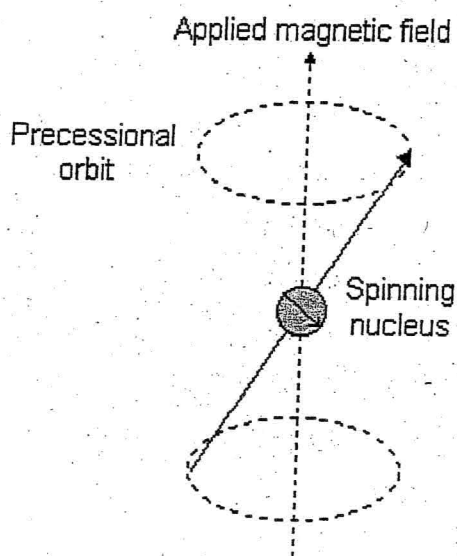
This means that if the magnetic field, B , is increased, so is ΔE . It also means that if a nucleus has a relatively large magnetogyric ratio, then ΔE is correspondingly large.

If you had trouble understanding this section, try reading the next bit (The absorption of radiation by a nucleus in a magnetic field) and then come back.

The absorption of radiation by a nucleus in a magnetic field

In this discussion, we will be taking a "classical" view of the behaviour of the nucleus - that is, the behaviour of a charged particle in a magnetic field.

Imagine a nucleus (of spin 1/2) in a magnetic field. This nucleus is in the lower energy level (i.e. its magnetic moment does not oppose the applied field). The nucleus is spinning on its axis. In the presence of a magnetic field, this axis of rotation will *precess* around the magnetic field;



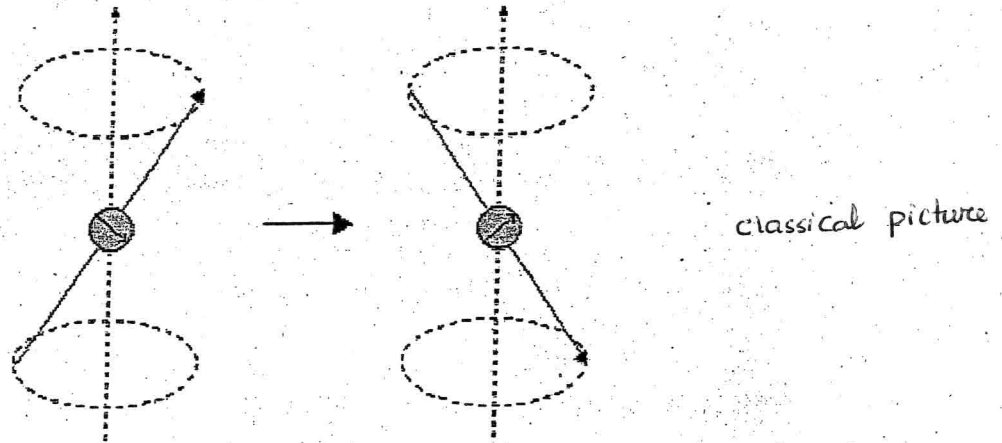
The frequency of precession is termed the Larmor frequency, which is identical to the transition frequency.

The potential energy of the precessing nucleus is given by;

$$E = -\mu B \cos \theta$$

where θ is the angle between the direction of the applied field and the axis of nuclear rotation.

If energy is absorbed by the nucleus, then the angle of precession, θ , will change. For a nucleus of spin $1/2$, absorption of radiation "flips" the magnetic moment so that it **opposes** the applied field (the higher energy state).



It is important to realise that only a small proportion of "target" nuclei are in the lower energy state (and can absorb radiation). There is the possibility that by exciting these nuclei, the populations of the higher and lower energy levels will become equal. If this occurs, then there will be **no** further absorption of radiation. The spin system is *saturated*. The possibility of saturation means that we must be aware of the relaxation processes which return nuclei to the lower energy state.

The following features lead to the NMR phenomenon:

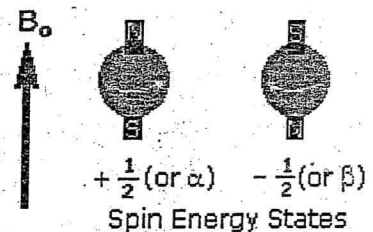
1. A spinning charge generates a magnetic field, as shown by the animation on the right.

The resulting spin-magnet has a magnetic moment (μ) proportional to the spin.

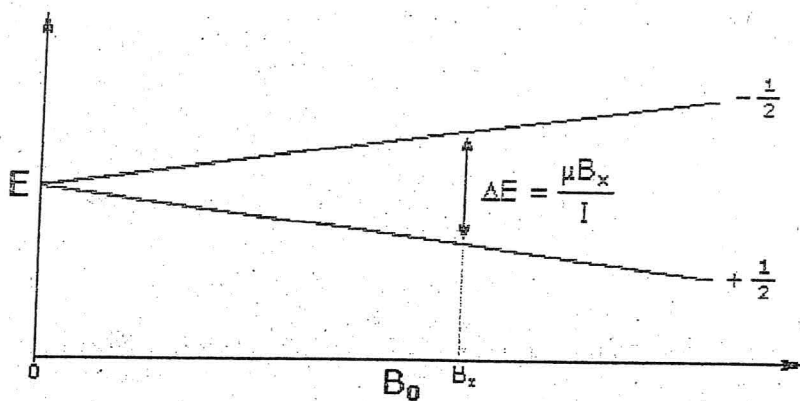


2. In the presence of an external magnetic field (B_0), two spin states exist, $+1/2$ and $-1/2$.

The magnetic moment of the lower energy $+1/2$ state is aligned with the external field, but that of the higher energy $-1/2$ spin state is opposed to the external field. Note that the arrow representing the external field points North.



3. The difference in energy between the two spin states is dependent on the external magnetic field strength, and is always very small. The following diagram illustrates that the two spin states have the same energy when the external field is zero, but diverge as the field increases. At a field equal to B_x a formula for the energy difference is given (remember $I = 1/2$ and μ is the magnetic moment of the nucleus in the field).

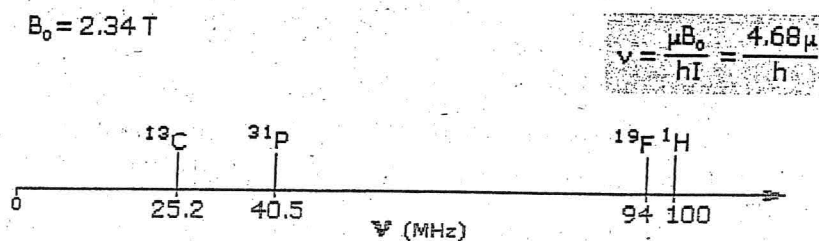


Strong magnetic fields are necessary for NMR spectroscopy. The international unit for magnetic flux is the tesla (T). The earth's magnetic field is not constant, but is approximately 10^{-4} T at ground level. Modern NMR spectrometers use powerful magnets having fields of 1 to 20 T. Even with these high fields, the energy difference between the two spin states is less than 0.1 cal/mole. To put this in perspective, recall that infrared transitions involve 1 to 10 kcal/mole and electronic transitions are nearly 100 times greater.

For nmr purposes, this small energy difference (ΔE) is usually given as a frequency in units of MHz (10^6 Hz), ranging from 20 to 900 Mz, depending on the magnetic field strength and the specific nucleus being studied. Irradiation of a sample with radio frequency (rf) energy corresponding exactly to the spin state separation of a specific set of nuclei will cause excitation of those nuclei in the $+1/2$ state to the higher $-1/2$ spin state. Note that this electromagnetic radiation falls in the radio and television broadcast spectrum. NMR spectroscopy is therefore the energetically mildest probe used to examine the structure of molecules.

The nucleus of a hydrogen atom (the proton) has a magnetic moment $\mu = 2.7927$, and has been studied more than any other nucleus. ~~The previous diagram may be changed to display energy differences for the proton spin states (as frequencies) by mouse clicking anywhere within it.~~

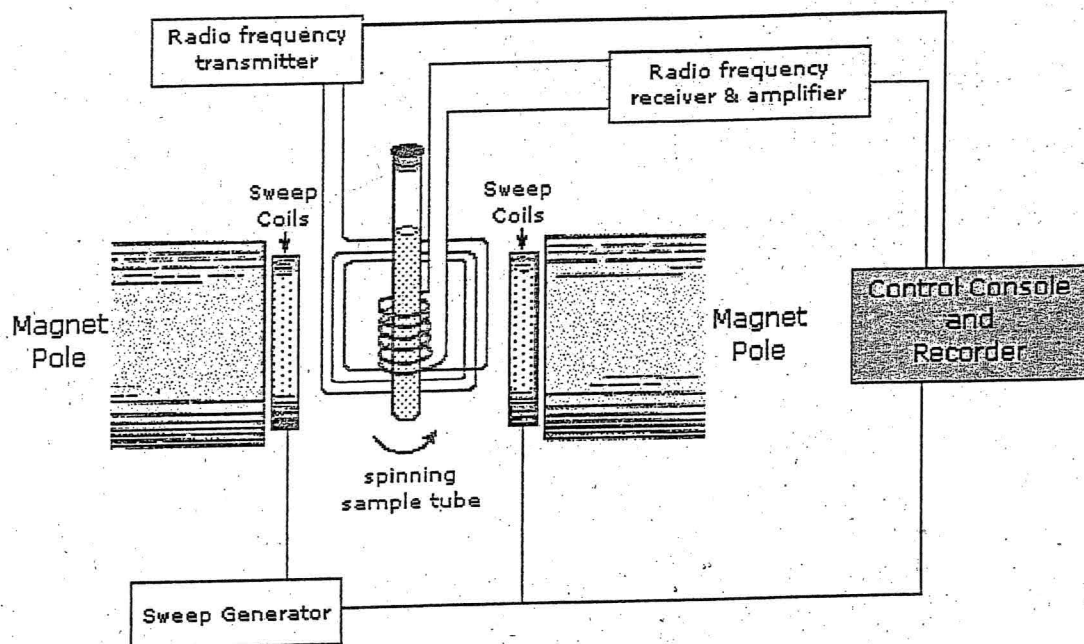
4. For spin $1/2$ nuclei the energy difference between the two spin states at a given magnetic field strength will be proportional to their magnetic moments. For the four common nuclei noted above the magnetic moments are: $^1\text{H } \mu = 2.7927$, $^{19}\text{F } \mu = 2.6273$, $^{31}\text{P } \mu = 1.1305$ & $^{13}\text{C } \mu = 0.7022$. The following diagram gives the approximate frequencies that correspond to the spin state energy separations for each of these nuclei in an external magnetic field of 2.34 T. The formula in the colored box shows the direct correlation of frequency (energy difference) with magnetic moment ($h = \text{Planck's constant}$).



2. Proton NMR Spectroscopy

This important and well-established application of nuclear magnetic resonance will serve to illustrate some of the novel aspects of this method. To begin with, the nmr spectrometer must be tuned to a specific nucleus, in this case the proton. The actual procedure for obtaining the spectrum varies, but the simplest is referred to as the **continuous wave (CW)** method. A typical CW-spectrometer is shown in the following diagram. A solution of the sample in a uniform 5 mm glass tube is oriented between the

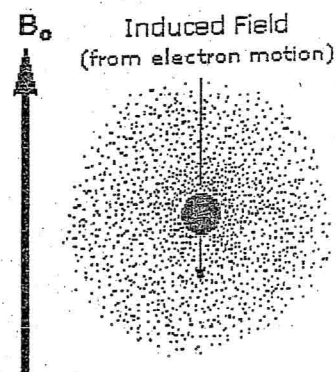
poles of a powerful magnet, and is spun to average any magnetic field variations, as well as tube imperfections. Radio frequency radiation of appropriate energy is broadcast into the sample from an antenna coil (colored red). A receiver coil surrounds the sample tube, and emission of absorbed rf energy is monitored by dedicated electronic devices and a computer. An nmr spectrum is acquired by varying or sweeping the magnetic field over a small range while observing the rf signal from the sample. An equally effective technique is to vary the frequency of the rf radiation while holding the external field constant.



Since protons all have the same magnetic moment, we might expect all hydrogen atoms to give resonance signals at the same field / frequency values. Fortunately for chemistry applications, this is not true. By clicking the **Show Different Protons** button under the diagram, a number of representative proton signals will be displayed over the same magnetic field range. It is not possible, of course, to examine isolated protons in the spectrometer described above; but from independent measurement and calculation it has been determined that a naked proton would resonate at a lower field strength than the nuclei of covalently bonded hydrogens. With the exception of water, chloroform and sulfuric acid, which are examined as liquids, all the other compounds are measured as gases.

Why should the proton nuclei in different compounds behave differently in the nmr experiment ?

The answer to this question lies with the electron(s) surrounding the proton in covalent compounds and ions. Since electrons are charged particles, they move in response to the external magnetic field (B_0) so as to generate a secondary field that opposes the much stronger applied field. This secondary field **shields** the nucleus from the applied field, so B_0 must be increased in order to achieve resonance (absorption of rf energy). As illustrated in the drawing on the right, B_0 must be increased to compensate for the induced shielding field. In the upper diagram, those compounds that give resonance signals at the higher field side of the diagram (CH_4 , HCl , HBr and HI) have proton nuclei that are more shielded than those on the lower field (left) side of the diagram.



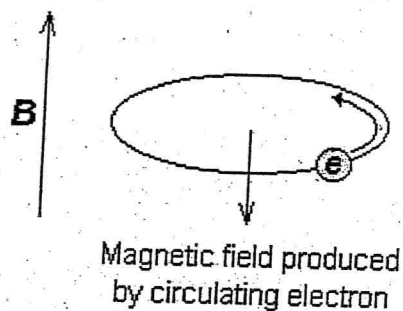
The magnetic field range displayed in the above diagram is very small compared with the actual field strength (only about 0.0042%). It is customary to refer to small increments such as this in units of **parts per million (ppm)**. The difference between 2.3487 T and 2.3488 T is therefore about 42 ppm. Instead

of designating a range of nmr signals in terms of magnetic field differences (as above), it is more common to use a frequency scale, even though the spectrometer may operate by sweeping the magnetic field. Using this terminology, we would find that at 2.34 T the proton signals shown above extend over a 4,200 Hz range (for a 100 MHz rf frequency, 42 ppm is 4,200 Hz). Most organic compounds exhibit proton resonances that fall within a 12 ppm range (the shaded area), and it is therefore necessary to use very sensitive and precise spectrometers to resolve structurally distinct sets of hydrogen atoms within this narrow range. In this respect it might be noted that the detection of a part-per-million difference is equivalent to detecting a 1 millimeter difference in distances of 1 kilometer.

Chemical Shift

The magnetic field at the nucleus is **not** equal to the applied magnetic field; electrons around the nucleus shield it from the applied field. The difference between the applied magnetic field and the field at the nucleus is termed the *nuclear shielding*.

Consider the s-electrons in a molecule. They have spherical symmetry and circulate in the applied field, producing a magnetic field which opposes the applied field. This means that the applied field strength must be increased for the nucleus to absorb at its transition frequency. This *upfield shift* is also termed *diamagnetic shift*.



Electrons in p-orbitals have **no** spherical symmetry. They produce comparatively large magnetic fields at the nucleus, which give a *low field shift*. This "deshielding" is termed *paramagnetic shift*.

In proton (^1H) NMR, p-orbitals play no part (there aren't any!), which is why only a small range of chemical shift (10 ppm) is observed. We can easily see the effect of s-electrons on the chemical shift by looking at substituted methanes, CH_3X . As X becomes increasingly electronegative, so the electron density around the protons decreases, and they resonate at lower field strengths (increasing δ_{H} values).

Chemical shift is defined as *nuclear shielding / applied magnetic field*. Chemical shift is a function of the nucleus and its environment. It is measured relative to a reference compound. For ^1H NMR, the reference is usually tetramethylsilane, $\text{Si}(\text{CH}_3)_4$.

Unlike infrared and uv-visible spectroscopy, where absorption peaks are uniquely located by a frequency or wavelength, the location of different NMR resonance signals is dependent on both the external magnetic field strength and the rf frequency. Since no two magnets will have exactly the same field, resonance frequencies will vary accordingly and an alternative method for characterising and specifying the location of NMR signals is needed. This problem is illustrated by the eleven different compounds shown in the following diagram. Although the eleven resonance signals are distinct and well separated, an unambiguous numerical locator cannot be directly assigned to each.

Chemical Shift

- ⇒ All protons should resonate at the same frequency
- ⇒ Electrons act to cancel part of the magnetic field
- ⇒ $H_{\text{effective}} = H_{\text{applied}} - H_{\text{local}}$
- ⇒ Each proton will resonate at a slightly different frequency depending on the electron density around it

Tetramethylsilane

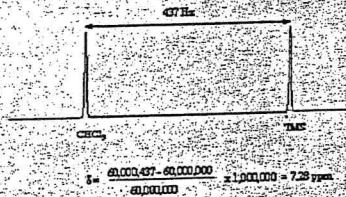
- ⇒ We need a reference peak to measure from
- ⇒ The most highly shielded protons are in tetramethylsilane



- ⇒ By definition TMS is 0.00. Everything is "down field" from TMS.

Chemical Shift (cont.)

- ⇒ Chloroform

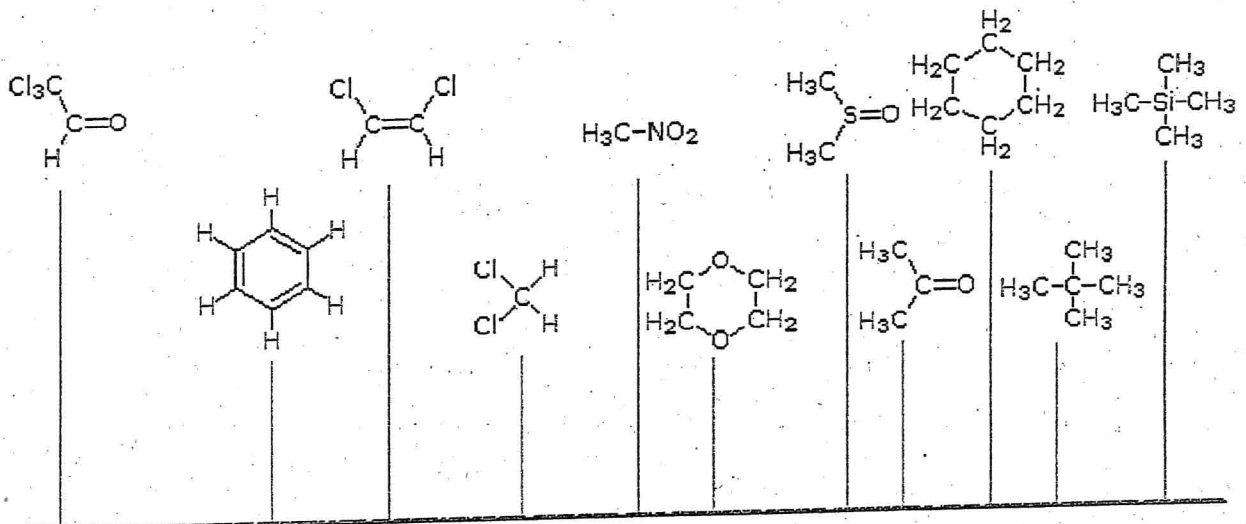


Chemical Shift (cont.)

- ⇒ All peaks are measured relative to TMS which is defined as 0
- ⇒ Chemical shifts in ppm are the same regardless of the magnet strength
- CHCl₃ on a 300 MHz machine is 2184 Hz from TMS

$$\delta = \frac{2184 \text{ Hz}}{300,000,000 \text{ Hz}} \times 10^6 = 7.28 \text{ ppm}$$

- Increasing Magnetic Field at Fixed Frequency →
- ← Increasing Frequency at Fixed Magnetic Field ←
- Increased Shielding by Extranuclear electrons →



¹H NMR Resonance Signals for some Different Compounds

One method of solving this problem is to report the location of an NMR signal in a spectrum relative to a reference signal from a standard compound added to the sample. Such a reference standard should be chemically unreactive, and easily removed from the sample after the measurement. Also, it should

give a single sharp NMR signal that does not interfere with the resonances normally observed for organic compounds. **Tetramethylsilane**, $(\text{CH}_3)_4\text{Si}$, usually referred to as **TMS**, meets all these characteristics, and has become the reference compound of choice for proton and carbon nmr. Since the separation (or dispersion) of nmr signals is magnetic field dependent, one additional step must be taken in order to provide an unambiguous location unit. To correct these frequency differences for their field dependence, we divide them by the spectrometer frequency (100 or 500 MHz in the example). The resulting number would be very small, since we are dividing Hz by MHz, so it is multiplied by a million, as shown by the formula in the blue shaded box. Note that ν_{ref} is the resonant frequency of the reference signal and ν_{samp} is the frequency of the sample signal. This operation gives a locator number called the **Chemical Shift**, having units of parts-per-million (ppm), and designated by the symbol δ .

The compounds referred to above share two common characteristics:

- The hydrogen atoms in a given molecule are all structurally equivalent, averaged for fast conformational equilibria.
- The compounds are all liquids, save for neopentane which boils at 9 °C and is a liquid in an ice bath.

The first feature assures that each compound gives a single sharp resonance signal. The second allows the pure (neat) substance to be poured into a sample tube and examined in a nmr spectrometer. In order to take the nmr spectra of a solid, it is usually necessary to dissolve it in a suitable solvent. Early studies used carbon tetrachloride for this purpose, since it has no hydrogen that could introduce an interfering signal. Unfortunately, CCl_4 is a poor solvent for many polar compounds and is also toxic. Deuterium labeled compounds, such as deuterium oxide (D_2O), chloroform-d (DCCl_3), benzene- d_6 (C_6D_6), acetone- d_6 (CD_3COCD_3) and DMSO- d_6 (CD_3SOCD_3) are now widely used as nmr solvents. Since the deuterium isotope of hydrogen has a different magnetic moment and spin, it is invisible in a spectrometer tuned to protons.

Properties of Some Deuterated NMR Solvents

Solvent	B.P. °C	Residual ^1H signal (δ)	Residual ^{13}C signal (δ)
acetone- d_6	55.5	2.05 ppm	206 & 29.8 ppm
acetonitrile- d_3	80.7	1.95 ppm	118 & 1.3 ppm
benzene- d_6	79.1	7.16 ppm	128 ppm
chloroform-d	60.9	7.27 ppm	26.4 ppm
cyclohexane- d_{12}	78.0	1.38 ppm	26.4 ppm
dichloromethane- d_2	40.0	5.32 ppm	53.8 ppm
dimethylsulfoxide- d_6	190	2.50 ppm	39.5 ppm
nitromethane- d_3	100	4.33 ppm	62.8 ppm
pyridine- d_5	114	7.19, 7.55 & 8.71 ppm	150, 135.5 & 123.5 ppm
tetrahydrofuran- d_8	65.0	1.73 & 3.58 ppm	67.4 & 25.2 ppm

From the previous discussion and examples we may deduce that one factor contributing to chemical shift differences in proton resonance is the inductive effect. If the electron density about a proton

nucleus is relatively high, the induced field due to electron motions will be stronger than if the electron density is relatively low. The shielding effect in such high electron density cases will therefore be larger, and a higher external field (B_0) will be needed for the rf energy to excite the nuclear spin. Since silicon is less electronegative than carbon, the electron density about the methyl hydrogens in tetramethylsilane is expected to be greater than the electron density about the methyl hydrogens in neopentane (2,2-dimethylpropane), and the characteristic resonance signal from the silane derivative does indeed lie at a higher magnetic field. Such nuclei are said to be **shielded**. Elements that are more electronegative than carbon should exert an opposite effect (reduce the electron density); and, as the data in the following tables show, methyl groups bonded to such elements display lower field signals (they are **deshielded**). The deshielding effect of electron withdrawing groups is roughly proportional to their electronegativity, as shown by the left table. Furthermore, if more than one such group is present, the deshielding is additive (table on the right), and proton resonance is shifted even further downfield.

Proton Chemical Shifts of Methyl Derivatives

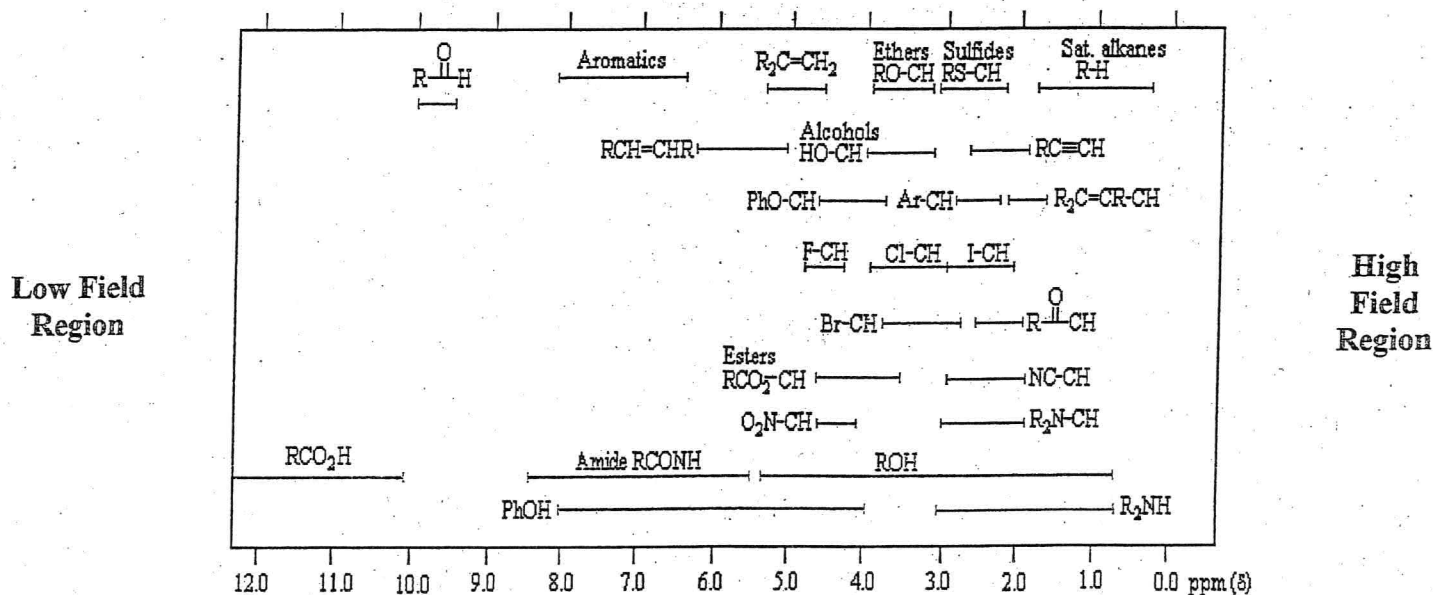
Compound	$(\text{CH}_3)_4\text{C}$	$(\text{CH}_3)_3\text{N}$	$(\text{CH}_3)_2\text{O}$	CH_3F
Δ	0.9	2.1	3.2	4.1
Compound	$(\text{CH}_3)_4\text{Si}$	$(\text{CH}_3)_3\text{P}$	$(\text{CH}_3)_2\text{S}$	CH_3Cl
Δ	0.0	0.9	2.1	3.0

Proton Chemical Shifts (ppm)

Cpd. / Sub.	X=Cl	X=Br	X=I	X=OR	X=SR
CH_3X	3.0	2.7	2.1	3.1	2.1
CH_2X_2	5.3	5.0	3.9	4.4	3.7
CHX_3	7.3	6.8	4.9	5.0	

The general distribution of proton chemical shifts associated with different functional groups is summarized in the following chart. Bear in mind that these ranges are approximate, and may not encompass all compounds of a given class. Note also that the ranges specified for OH and NH protons (colored orange) are wider than those for most CH protons. This is due to hydrogen bonding variations at different sample concentrations.

Proton Chemical Shift Ranges*



* For samples in CDCl_3 solution. The δ scale is relative to TMS at $\delta = 0$.

1. PHYSICAL CONSTANTS

Table 1.1. Reviewed 2004 by P.J. Mohr and B.N. Taylor (NIST). Based mainly on the "CODATA Recommended Values of the Fundamental Physical Constants: 2002" by P.J. Mohr and B.N. Taylor, to be published in 2004. The last group of constants (beginning with the Fermi coupling constant) comes from the Particle Data Group. The figures in parentheses after the values give the 1-standard-deviation uncertainties in the last digits; the corresponding fractional uncertainties in parts per 10⁹ (ppb) are given in the last column. This set of constants (aside from the last group) is recommended for international use by CODATA (the Committee on Data for Science and Technology). The full 2002 CODATA set of constants may be found at <http://physics.nist.gov/constants>

Quantity	Symbol, equation	Value	Uncertainty (ppb)
speed of light in vacuum	c	299 792 458 m s ⁻¹	exact*
Planck constant	h	6.626 0693(11) × 10 ⁻³⁴ J s	170
Planck constant, reduced	$\hbar \equiv h/2\pi$	1.054 571 68(18) × 10 ⁻³⁴ J s = 6.582 119 15(56) × 10 ⁻²² MeV s	170
electron charge magnitude	e	1.602 176 53(14) × 10 ⁻¹⁹ C = 4.803 204 41(41) × 10 ⁻¹⁰ esu	85, 85
conversion constant	$\hbar c$	197.326 968(17) MeV fm	85
conversion constant	$(\hbar c)^2$	0.389 379 323(67) GeV ² mbarn	170
electron mass	m_e	0.510 998 918(44) MeV/c ² = 9.109 3826(16) × 10 ⁻³¹ kg	86, 170
proton mass	m_p	938.272 029(80) MeV/c ² = 1.672 621 71(29) × 10 ⁻²⁷ kg = 1.007 276 466 88(13) u = 1836.152 672 61(85) m _e	86, 170
deuteron mass	m_d	1875.612 82(16) MeV/c ²	0.13, 0.46
unified atomic mass unit (u)	(mass ¹² C atom)/12 = (1 g)/(N _A mol)	931.494 043(80) MeV/c ² = 1.660 538 86(28) × 10 ⁻²⁷ kg	86, 170
permittivity of free space	$\epsilon_0 = 1/\mu_0 c^2$	8.854 187 817 ... × 10 ⁻¹² F m ⁻¹	exact
permeability of free space	μ_0	4π × 10 ⁻⁷ N A ⁻² = 12.566 370 614 ... × 10 ⁻⁷ N A ⁻²	exact
fine-structure constant	$\alpha = e^2/4\pi\epsilon_0\hbar c$	7.297 352 568(24) × 10 ⁻³ = 1/137.035 999 11(46) [†]	3.3, 3.3
classical electron radius	$r_e = e^2/4\pi\epsilon_0 m_e c^2$	2.817 940 325(28) × 10 ⁻¹⁵ m	10
(e ⁻ Compton wavelength)/2π	$\lambda_e = h/m_e c = r_e \alpha^{-1}$	3.861 592 678(26) × 10 ⁻¹³ m	6.7
Bohr radius (m _{nucleus} = ∞)	$a_\infty = 4\pi\epsilon_0 \hbar^2 / m_e e^2 = r_e \alpha^{-2}$	0.529 177 2108(18) × 10 ⁻¹⁰ m	3.3
wavelength of 1 eV/c particle	$hc/(1 \text{ eV})$	1.239 841 91(11) × 10 ⁻⁶ m	85
Rydberg energy	$hcR_\infty = m_e e^4 / 2(4\pi\epsilon_0)^2 \hbar^2 = m_e c^2 \alpha^2 / 2$	13.605 6923(12) eV	85
Thomson cross section	$\sigma_T = 8\pi r_e^2 / 3$	0.665 245 873(13) barn	20
Bohr magneton	$\mu_B = e\hbar/2m_e$	5.788 381 804(39) × 10 ⁻¹¹ MeV T ⁻¹	6.7
nuclear magneton	$\mu_N = e\hbar/2m_p$	3.152 451 259(21) × 10 ⁻¹⁴ MeV T ⁻¹	6.7
electron cyclotron freq./field	$\omega_{\text{cycl}}^e / B = e/m_e$	1.758 820 12(15) × 10 ¹¹ rad s ⁻¹ T ⁻¹	86
proton cyclotron freq./field	$\omega_{\text{cycl}}^p / B = e/m_p$	9.578 833 76(82) × 10 ⁷ rad s ⁻¹ T ⁻¹	86
gravitational constant [‡]	G_N	6.6742(10) × 10 ⁻¹¹ m ³ kg ⁻¹ s ⁻² = 6.7087(10) × 10 ⁻³⁹ ħc (GeV/c ²) ⁻²	1.5 × 10 ⁵ 1.5 × 10 ⁵
standard gravitational accel.	g_n	9.806 65 m s ⁻²	exact
Avogadro constant	N_A	6.022 1415(10) × 10 ²³ mol ⁻¹	170
Boltzmann constant	k	1.380 6505(24) × 10 ⁻²³ J K ⁻¹ = 8.617 343(15) × 10 ⁻⁵ eV K ⁻¹	1800
molar volume, ideal gas at STP	$N_A k(273.15 \text{ K})/(101.325 \text{ Pa})$	22.413 996(39) × 10 ⁻³ m ³ mol ⁻¹	1800
Wien displacement law constant	$b = \lambda_{\text{max}} T$	2.897 7685(51) × 10 ⁻³ m K	1700
Stefan-Boltzmann constant	$\sigma = \pi^2 k^4 / 60\hbar^3 c^2$	5.670 400(40) × 10 ⁻⁸ W m ⁻² K ⁻⁴	7000
Fermi coupling constant**	$G_F/(\hbar c)^3$	1.166 37(1) × 10 ⁻⁵ GeV ⁻²	9000
weak-mixing angle	$\sin^2 \hat{\theta}(M_Z)$ (MS)	0.23120(15) ^{††}	6.5 × 10 ⁵
W [±] boson mass	m_W	80.425(38) GeV/c ²	4.8 × 10 ⁵
Z ⁰ boson mass	m_Z	91.1876(21) GeV/c ²	2.3 × 10 ⁴
strong coupling constant	$\alpha_s(m_Z)$	0.1187(20)	1.7 × 10 ⁷
$\pi = 3.141 592 653 589 793 238$		$e = 2.718 281 828 459 045 235$	$\gamma = 0.577 215 664 901 532 861$
1 in ≡ 0.0254 m	1 G ≡ 10 ⁻⁴ T	1 eV = 1.602 176 53(14) × 10 ⁻¹⁹ J	kT at 300 K = [38.681 684(68)] ⁻¹ eV
1 Å ≡ 0.1 nm	1 dyne ≡ 10 ⁻⁵ N	1 eV/c ² = 1.782 661 81(15) × 10 ⁻³⁶ kg	0 °C ≡ 273.15 K
1 barn ≡ 10 ⁻²⁸ m ²	1 erg ≡ 10 ⁻⁷ J	2.997 924 58 × 10 ⁹ esu = 1 C	1 atmosphere ≡ 760 Torr ≡ 101 325 Pa

* The meter is the length of the path traveled by light in vacuum during a time interval of 1/299 792 458 of a second. At Q² = 0. At Q² ≈ m_W², the value is ~ 1/128.

† Absolute lab measurements of G_N have been made only on scales of about 1 cm to 1 m.

** See the discussion in Sec. 10, "Electroweak model and constraints on new physics."

†† The corresponding sin² θ for the effective angle is 0.23149(15).

NMR

Calculation

At resonance,

$$\Delta E = \frac{\gamma h B}{2\pi} = h\nu$$

↳ Energy of photon

γ = Gyromagnetic ratio

ν = Resonance freq.

$$\Rightarrow \nu_{res} = \frac{\gamma B}{2\pi}$$

For Glycerine (Proton NMR),

$$\gamma_{H_2} = 26.752 \times 10^7 \text{ rad s}^{-1} \text{ T}^{-1}$$

(i) Calculate $B = ?$ for known ν_{res} (from expt.) with error

(ii) Lande-g-factor = $g = \frac{\gamma h}{\mu_N} = \frac{\gamma 2 m_p}{e}$; $\gamma = \gamma_{H_2}$ (known from literature)

[Compare with literature value of g]

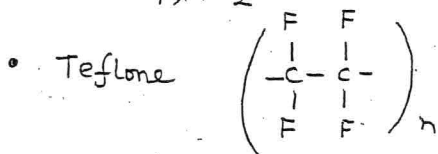
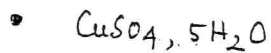
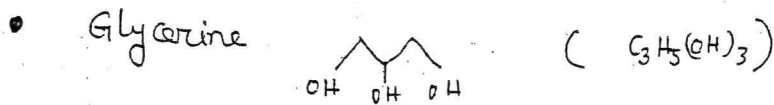
For rest samples,

$B = \text{known}$

$\nu_{res} = \text{known (from expt.)}$

i) Find out Gyromagnetic ratio = γ
& calculate g

Compare with literature value



Landé g-factor

In physics, the **Landé g-factor** is a particular example of a g-factor, namely for an electron with both spin and orbital angular momenta. It is named after Alfred Landé, who first described it in 1921.

In atomic physics, it is a multiplicative term appearing in the expression for the energy levels of an atom in a weak magnetic field. The quantum states of electrons in atomic orbitals are normally degenerate in energy, with the degenerate states all sharing the same angular momentum. When the atom is placed in a weak magnetic field, however, the degeneracy is lifted.

The factor comes about during the calculation of the first-order perturbation in the energy of an atom when a weak uniform magnetic field (that is, weak in comparison to the system's internal magnetic field) is applied to the system. Formally we can write the factor as,

$$g_J = g_L \frac{J(J+1) - S(S+1) + L(L+1)}{2J(J+1)} + g_S \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

$$\approx 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

$$g_L = 1, g_S \approx 2$$

Here, J is the total electronic angular momentum, L is the orbital angular momentum, and S is the spin angular momentum. Because $S=1/2$ for electrons, one often sees this formula written with $3/4$ in place of $S(S+1)$. The quantities g_L and g_S are other g-factors of an electron.

If we wish to know the g-factor for an atom with total atomic angular momentum $F=I+J$,

$$g_F = g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)} + g_I \frac{F(F+1) + I(I+1) - J(J+1)}{2F(F+1)}$$

$$\approx g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)}$$

This last approximation is justified because g_I is smaller than g_J by the ratio of the electron mass to the proton mass.

Kurzcheck-Protokoll

1. Theoretischer Hintergrund inklusive Formeln und Diagrammen
2. Versuchsaufbau
3. Resultate und Auswertungen:
 - a. Magnetische Feldwerte B_{max} und B_{min}
 - b. g-Faktor und gyromagnetisches Verhältnis γ
 - c. Identifizierung der untersuchten Kernmomente
4. Explizite Fehlerrechnung
5. Anwendungen der NMR
6. Schlussfolgerungen

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