Terminology Commonly Used in NMR Spectroscopy

**absolute intensity**
A display or plot mode in which the signal intensity is proportional to the concentration of the species producing it.

**acquisition time**
Time during which signal is recorded (see figure 1).

![Figure 1. Signal is acquired in the time domain.](image)

**attenuation**
The control applied to voltages (including signal from the sample) within the spectrometer. High attenuation gives low-voltage, low-attenuation gives high-voltage.

**B₀**
The static magnetic field. The magnetic flux density is expressed in tesla, T, or often, as an equivalent $^1$H resonance frequency (for example, 300 MHz for a 7 T magnet).

**B₁**
Magnetic field associated with a radio-frequency (r.f.) pulse. Often expressed as an equivalent value in kHz.

**bandshape**
Usually used when referring to a complex lineshape or a group of overlapping lines. Complex bandshapes often arise from quadrupolar nuclei (see figure 2).

**centreband**
The signal at the isotropic chemical shift. Its position is the same at all spin-rates.

**channel**
The individual frequencies or frequency bands of a spectrometer. For example: H-channel (proton), C-channel (carbon) or broad-band (or X) channel (usually anything except H).

**chemical shift**
Number used for reporting the position of a line ($ν_i$) relative to a reference line ($ν_{ref}$) in a high-resolution spectrum. The chemical shift parameter is denoted $δ$ and quoted in ppm.

$$δ = \frac{ν_i - ν_{ref}}{ν_{ref}} \times 10^6$$

**coherence pathway**
Description of an experiment that allows the excitation of the spins to be followed. Useful for experiments where excitation or selection of signal from one-, two- or multiple-quantum transitions is needed.

**contact time**
Time during which two matched radio-frequency fields are applied simultaneously in a CP experiment.

**CP**
Cross-polarisation. Any experiment where energy (magnetisation) is transferred from the nuclei of one element (often H) to those of another.

**dead-time**
Time between a pulse and the switch on of the receiver. The spectrometer circuitry needs time to settle after transmitting the high voltage associated with a pulse before it can detect the very low voltage associated with the signal from the sample. See figure 1.

![Figure 2. Bandshape from a single $^1$B environment.](image)
<table>
<thead>
<tr>
<th>Term</th>
<th>Definition/Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>d.c. offset</td>
<td>Constant-value offset occurring in the FID (see “Problems”). Results in a central (zero-frequency) “spike” artefact in the spectrum when transformed.</td>
</tr>
<tr>
<td>deconvolution</td>
<td>Mathematical process used to determine the intensities of overlapping lines.</td>
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<tr>
<td>digital resolution</td>
<td>This depends on the Fourier number. The bigger the Fourier number the greater the number of data points per Hz of the spectrum and the higher the digital resolution. See “Processing”.</td>
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<tr>
<td>DP</td>
<td>Direct-polarisation. An experiment in which the nuclei to be observed are excited directly.</td>
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<tr>
<td>duty cycle</td>
<td>A value used to assess whether an experiment might damage the spectrometer (or the sample). The duty cycle should never exceed 20% (see “How to Choose a Recycle Delay”).</td>
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<tr>
<td>dwell</td>
<td>Spacing between data points in the time-domain. Can depend on the way acquisition is implemented but, commonly, dwell = 1 / spectral width.</td>
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<tr>
<td>endcap</td>
<td>Open rotors have to be closed with endcaps before they can be spun.</td>
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<tr>
<td>FID</td>
<td>Free Induction Decay (see figure 1).</td>
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<tr>
<td>field</td>
<td>Magnetic field, with flux density quoted in T (Tesla) for the static magnetic field ($B_0$). For the magnetic field associated with an r.f. pulse the flux density is given in mT or, more usually, expressed as a kHz equivalent (see “Matching”).</td>
</tr>
<tr>
<td>flip-back</td>
<td>Experimental procedure for shortening recycle times (see “How to Choose a Recycle”).</td>
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<tr>
<td>Fourier number</td>
<td>The number of points used in the FT. Always a power of 2.</td>
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<tr>
<td>frequency domain</td>
<td>Where information is displayed as a function of frequency - the spectrum.</td>
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<tr>
<td>FT</td>
<td>Fourier Transform. Mathematical process to convert time-domain to frequency-domain. Designed to work with $2^n$ ($n = \text{integer}$) data points.</td>
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<tr>
<td>gain</td>
<td>Amplification applied to the received signal.</td>
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<tr>
<td>Gauss</td>
<td>Non-SI unit of magnetic field flux density. The SI equivalent is Tesla (T), 1 T = 10,000 G.</td>
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<tr>
<td>intensity</td>
<td>On its own - the height of a line. Integrated-intensity is the area under the line.</td>
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<tr>
<td>linebroadening</td>
<td>Spectra can be artificially linebroadened to improve their appearance. This involves multiplying the FID with a decaying function prior to the FT. See “Processing”.</td>
</tr>
<tr>
<td>lineshape</td>
<td>The shape of individual lines in a spectrum. Commonly, Gaussian or Lorentzian (figure 3) or a mixture of the two, are encountered experimentally.</td>
</tr>
<tr>
<td>linewidth</td>
<td>This is usually the full width at half-height ($\delta\nu_{1/2}$)</td>
</tr>
</tbody>
</table>
magic-angle 54.7° or 54° 44´
magnetisation when described classically (non-quantum mechanically) an ensemble of spins at equilibrium in an external magnetic field has a net magnetisation precessing about an axis aligned along that field.
magnetogyric ratio Symbol $\gamma$. A fundamental physical constant of elements with non-zero spin. For example $\gamma_H$ is $2.675 \times 10^8 \text{ rads}^{-1} \text{T}^{-1}$.
normalised intensity Signal intensity can be multiplied by an arbitrary factor to give a particular height to the highest (often) line or the integrated intensity. Opposite of absolute intensity.
nuclear spin quantum number Symbol $I$. A fundamental property of a nucleus. Only nuclei with $I > 0$ are said to be NMR “active”.

phase (1) The phase of a pulse relates to its position in the xy plane of the rotating frame.
phase (2) The phase of a spectral line comes from the way in which the real and imaginary components of a complex FT are combined (see “Processing”).
phase cycling The way in which the phase of a pulse (or the receiver) is changed during successive repetitions of a pulse sequence. Used to suppress artefacts and select specific coherence pathways.
ppm Parts per million. Usual way of reporting a chemical shift. A frequency difference $\Delta \approx 6 \times 10^6 \text{ ppm}$
precession “Movement of the axis of a spinning body around another axis” (as a gyroscope)
probe The business end of the spectrometer, where the sample goes.
pulse angle When described in the rotating frame a pulse rotates the magnetisation through an angle $\theta$. A pulse that rotates the magnetisation through 90° is called a 90° pulse.
pulse duration Time for which a pulse occurs.
quadrupole Any nucleus with $I > \frac{1}{2}$.
recycle (time) Or pulse delay or relaxation delay. Time between the end of data acquisition and the start of excitation in successive repetitions of a pulse sequence. (See “How to Choose a Recycle”).
reference The material giving the signal which defines the zero position in a high-
resolution spectrum.

**repetitions**

The number of times a pulse sequence is repeated in an experiment.

**resolution**

The ability to separate closely spaced lines (see figure 4). As a rule of thumb, a pair of lines will be resolved if their linewidth is less than their separation.

**resolution enhancement**

The opposite of linebroadening. An FID multiplied by an appropriate combination of increasing and decaying functions can yield extra resolution in a spectrum. See “Processing”.

**rotary echo**

A feature of an FID that occurs at intervals of 1/spin-rate (see “How to Set the Magic-angle”). They give rise to spinning sidebands in the spectrum.

**rotating frame**

A mathematical tool to make the effect of a pulse easy to visualise. Magnetisation precessing at ν Hz in a laboratory-based xz axis system appears static in an axis system (frame) rotating at ν Hz.

**rotor**

The container that holds the sample. Often referred to in terms of its outside diameter (for example, 5 mm).

**saturation**

Condition that arises when there is no population difference between excited and ground states. No signal is observable under such conditions.

**sidebands**

Or spinning sidebands. Under some circumstances sidebands appear in a spectrum. They can occur on both sides of a centreband and separated from it by a frequency equal to the spin-rate. A spectrum may contain a manifold of sidebands and the centreband is not necessarily more intense than all of the sidebands.

**signal**

The FID or one or more of the lines in a spectrum.

**signal-to-noise ratio (S/N)**

Ratio of the height of a line or signal (usually the largest) to the noise. Definitions of the measurement of noise vary. Signal increases as n (the number of repetitions) but noise only increases by √n so S/N increases by √n.

**spectral width**

Difference in frequency of the two ends of the full spectrum. Not to be confused with the now largely obsolete term sweep width.

**spin**

A property of a nucleus with non-zero nuclear spin-quantum number (I), as in spin-½. Or, simply, a nucleus with a magnetic moment.

**spin-lock**

If, after a 90° pulse a second, long-duration (spin-lock) r.f. field is applied along the y-axis the magnetisation is said to be spin-locked.

**spin-rate**

The rate at which the sample is spun.

**spin-temperature inversion**

A manipulation carried out within the phase cycling of a CP experiment to remove magnetisation originating directly from the X-channel contact pulse.

**standard**

Any sample used to set-up the spectrometer and/or to define the zero position in the spectrum.

Figure 4. Two lines of constant spacing but different linewidth.
$T_1$  
Spin-lattice relaxation time-constant. Relates to the time taken for excited spins, in the presence of $B_0$, to lose energy to their surroundings and return to their equilibrium state.

$T_{1\rho}$  
Spin-lattice relaxation time-constant in the rotating frame. As for $T_1$, but this time in the presence of an applied radio-frequency field $B_1$.

$T_2$  
Spin-spin relaxation time-constant. Relates to the time for a conserved exchange of energy between spins.

$T^*_2$  
A time-constant sometimes used to describe the decay of the observed time-domain signal ($T^*_2 \leq T_2$). The shorter $T^*_2$ the broader the associated signal(s) in the spectrum.

_time-domain_
Where information is recorded or displayed as a function of time (see figure 1).

_transmitter offset_
This allows fine control of the position of a transmitter (carrier frequency). With an appropriate offset, signals can be put exactly on-resonance or a specific amount off-resonance. Can be applied to any spectrometer channel.

_truncation_
If the acquisition time is shorter than the FID then truncation of the FID is said to have occurred (See “Problems”).

_zero filling_
If the number of data points is not a power of two then zeroes are added to the acquired data so that the total number of points Fourier transformed is $2^n$. Zero filling adds no signal to the spectrum but it can improve resolution (see “Processing”).