



Standard Practice for Data Presentation Relating to High-Resolution Nuclear Magnetic Resonance (NMR) Spectroscopy¹

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1. Scope

1.1 This standard contains definitions of basic terms, conventions, and recommended practices for data presentation in the area of high-resolution NMR spectroscopy. Some of the basic definitions apply to wide-line NMR or to NMR of metals, but in general it is not intended to cover these latter areas of NMR in this standard. This version does not include definitions pertaining to double resonance nor to rotating frame experiments.

2. Terminology Nomenclature and Basic Definitions

2.1 *nuclear magnetic resonance (NMR) spectroscopy*—that form of spectroscopy concerned with radio-frequency-induced transitions between magnetic energy levels of atomic nuclei.

2.2 *NMR apparatus; NMR equipment*—an instrument comprising a magnet, radio-frequency oscillator, sample holder, and a detector that is capable of producing an electrical signal suitable for display on a recorder or an oscilloscope, or which is suitable for input to a computer.

2.3 *high-resolution NMR spectrometer*—an NMR apparatus that is capable of producing, for a given isotope, line widths that are less than the majority of the chemical shifts and coupling constants for that isotope.

NOTE 1—By this definition, a given spectrometer may be classed as a high-resolution instrument for isotopes with large chemical shifts, but may not be classed as a high-resolution instrument for isotopes with smaller chemical shifts.

2.4 *basic NMR frequency, ν_o* —the frequency, measured in hertz (Hz), of the oscillating magnetic field applied to induce transitions between nuclear magnetic energy levels. The static magnetic field at which the system operates is called H_o (Note 1) and its recommended unit of measurement is the tesla (T) ($1 \text{ T} = 10^4 \text{ gauss}$).

2.4.1 The foregoing quantities are approximately connected by the following relation:

$$\nu_o = \frac{\gamma}{2\pi} H_o \quad (1)$$

where γ = the magnetogyric ratio, a constant for a given

nuclide (Note 2). The amplitude of the magnetic component of the radio-frequency field is called H_1 . Recommended units are millitesla and microtesla.

NOTE 2—This quantity is normally referred to as B by physicists. The usage of H to refer to magnetic field strength in chemical applications is so widely accepted that there appears to be no point in attempting to reach a totally consistent nomenclature now.

NOTE 3—This expression is correct only for bare nuclei and will be only approximately true for nuclei in chemical compounds, since the field at the nucleus is in general different from the static magnetic field. The discrepancy amounts to a few parts in 10^6 for protons, but may be of magnitude 1×10^{-3} for the heaviest nuclei.

2.5 *NMR absorption line*—a single transition or a set of degenerate transitions is referred to as a line.

2.6 *NMR absorption band; NMR band*—a region of the spectrum in which a detectable signal exists and passes through one or more maxima.

2.7 *reference compound (NMR)*—a selected material to whose signal the spectrum of a sample may be referred for the measurement of chemical shift (see 2.9).

2.7.1 *internal reference (NMR)*—a reference compound that is dissolved in the same phase as the sample.

2.7.2 *external reference (NMR)*—a reference compound that is not dissolved in the same phase as the sample.

2.8 *lock signal*—the NMR signal used to control the field-frequency ratio of the spectrometer. It may or may not be the same as the reference signal.

2.8.1 *internal lock*—a lock signal which is obtained from a material that is physically within the confines of the sample tube, whether or not the material is in the same phase as the sample (an annulus for the purpose of this definition is considered to be within the sample tube).

2.8.2 *external lock*—a lock signal which is obtained from a material that is physically outside the sample tube. The material supplying the lock signal is usually built into the probe.

NOTE 4—An external lock, if also used as a reference, is necessarily an external reference. An internal lock, if used as a reference, may be either an internal or an external reference, depending upon the experimental configuration.

2.8.3 *homonuclear lock*—a lock signal which is obtained from the same nuclide that is being observed.

2.8.4 *heteronuclear lock*—a lock signal which is obtained from a different nuclide than the one being observed.

¹ These practices are under the jurisdiction of ASTM Committee E-13 on Molecular Spectroscopy and are the direct responsibility of Subcommittee E13.07 on Nuclear Magnetic Resonance Spectroscopy.

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