



Standard Practice for Measuring and Reporting Performance of Fourier-Transform Nuclear Magnetic Resonance (FT-NMR) Spectrometers for Liquid Samples¹

This standard is issued under the fixed designation E2977; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice covers procedures for measuring and reporting the performance of Fourier-transform nuclear magnetic resonance spectrometers (FT-NMRs) using liquid samples.

1.2 This practice is not directly applicable to FT-NMR spectrometers outfitted to measure gaseous, anisotropically structured liquid, semi-solid, or solid samples; those set up to work with flowing sample streams; or those used to make hyperpolarization measurements.

1.3 This practice was expressly developed for FT-NMR spectrometers operating with proton resonance frequencies between 200 and 1200 MHz.

1.4 This practice is not directly applicable to continuous wave (scanning) NMR spectrometers.

1.5 This practice is not directly applicable to instruments using single-sideband detection.

1.6 *Units*—The values stated in SI units are to be regarded as the standard. No other units of measurement are included in this standard.

1.7 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 ASTM Standards:²

E131 Terminology Relating to Molecular Spectroscopy

¹ This test method is under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Separation Science and is the direct responsibility of Subcommittee E13.15 on Analytical Data.

Current edition approved May 1, 2015. Published May 2015. Originally approved in 2014. Last previous edition approved in 2014 as E2977–14. DOI: 10.1520/E2977-15.

² For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

E386 Practice for Data Presentation Relating to High-Resolution Nuclear Magnetic Resonance (NMR) Spectroscopy

2.2 ISO Standard:³

ISO Guide 31 Reference Materials—Contents of Certificates and Labels

3. Terminology

3.1 *Definitions*—For definitions of terms used in this practice, refer to Terminology E131, Practice E386, and Refs (1-4).⁴ Chemical shifts are usually given in the dimensionless quantity, δ , commonly expressed in parts per million. For a given nucleus, the chemical shift scale is relative and is commonly pegged to the resonance of an agreed upon reference material as described by Eq 1.

$$\delta_{\text{sample}} = (v_{\text{sample}} - v_{\text{reference}}) \div v_{\text{reference}} \quad (1)$$

3.1.1 Frequencies are given in Hertz. Because the numerator is very small compared with the denominator, it is usually convenient to express δ in parts per million.

3.1.2 As the location of a resonance is determined in part by the ratio of the magnetic field to the radio frequency at which it is observed, chemical shifts and spectral regions are often designated as lower frequency (increased shielding) or higher frequency (decreased shielding) relative to a reference point. Defined in this manner, chemical shifts are independent of either the magnetic field or the radio frequency used. Coupling constants, which are independent of the magnetic field or radio frequency used, are expressed in Hertz.

3.1.3 *nuclear magnetic resonance (NMR) tube camber, n*—maximum total deflection of any part of the outer wall of the tube held at the ends and rotated 360°; a measure of the bow in the tube.

3.1.4 *NMR tube concentricity, n*—maximum variation in wall thickness of the tube; a measure of how centered the tube inside diameter is relative to the tube outer diameter.

³ Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, <http://www.ansi.org>.

⁴ The boldface numbers in parentheses refer to the list of references at the end of this standard.