



Standard Practice for Near Infrared Qualitative Analysis¹

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^{ε 1} NOTE—Editorial change was made in Subsection 6.6.3 in April 2016.

1. Scope

1.1 This practice covers the use of near-infrared (NIR) spectroscopy for the qualitative analysis of liquids and solids. The practice is written under the assumption that most NIR qualitative analyses will be performed with instruments designed specifically for this region and equipped with computerized data handling algorithms. In principle, however, the practice also applies to work with liquid samples using instruments designed for operation over the ultraviolet (UV), visible, and mid-infrared (IR) regions if suitable data handling capabilities are available. Many Fourier Transform Infrared (FTIR) (normally considered mid-IR instruments) have NIR capability, or at least extended-range beamsplitters that allow operation to 1.2 μm; this practice also applies to data from these instruments.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 *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

E1252 Practice for General Techniques for Obtaining Infrared Spectra for Qualitative Analysis

E1655 Practices for Infrared Multivariate Quantitative Analysis

¹ This practice is under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Separation Science and is the direct responsibility of Subcommittee E13.11 on Multivariate Analysis.

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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.

3. Terminology

3.1 *Definitions*—For definitions of general terms and symbols pertaining to NIR spectroscopy and statistical computations, refer to Terminology E131.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *interactance, n*—the phenomenon whereby radiant energy entering the surface of a material is scattered by the material back to the surface, but at a different portion of the surface.

3.2.1.1 *Discussion*—This differs from diffuse reflectance, where the returning radiation exits the same portion of the surface of the material as the illuminating radiation entered.

3.2.2 *training sample (otherwise called a “reference sample” or “standard”)*, *n*—a quantity of material of known composition or properties, or both, presented to an instrument for measurement in order to find relationships between the measurements and the composition or properties, or both, of the sample.

3.2.2.1 *Discussion*—This term is typically used in conjunction with computerized methods for ascertaining the relationships.

Training samples for quantitative analysis (also called “calibration samples,” as in Practices E1655) have different requirements than training samples used for qualitative analysis.

4. Significance and Use

4.1 NIR spectroscopy is a widely used technique for quantitative analysis, and it is also becoming more widely used for the identification of organic materials, that is, qualitative analysis. In general, however, the concept of qualitative analysis as used in the NIR spectral region differs from that used in the mid-IR spectral region in that NIR qualitative analysis refers to the process of automated comparison of the spectra of unknown materials to the spectra of known materials in order to identify the unknown. This approach constitutes a library search method in which each user generates his own library.

4.2 Historically, NIR spectroscopy as practiced with classical UV-VIS-NIR instruments using methods similar to those described in Practice E1252 was not considered to be a strong technique for qualitative analysis. Although the positions and