



Standard Practice for General Techniques for Obtaining Infrared Spectra for Qualitative Analysis¹

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1. Scope

1.1 This practice covers the spectral range from 4000–50 cm⁻¹ and includes techniques that are useful for qualitative analysis of liquid-, solid-, and vapor-phase samples by infrared spectrometric techniques for which the amount of sample available for analysis is not a limiting factor. These techniques are often also useful for recording spectra at frequencies higher than 4000 cm⁻¹, in the near-infrared region.

1.2 *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.* Specific precautions are given in 6.5.1.

2. Referenced Documents

2.1 ASTM Standards:

- E 131 Terminology Relating to Molecular Spectroscopy²
- E 168 Practices for General Techniques of Infrared Quantitative Analysis²
- E 334 Practices for General Techniques of Infrared Microanalysis²
- E 573 Practices for Internal Reflection Spectroscopy²
- E 932 Practice for Describing and Measuring Performance of Dispersive Infrared Spectrometers²
- E 1421 Practice for Describing and Measuring Performance of Fourier Transform Infrared (FT-IR) Spectrometers: Level Zero and Level One²
- E 1642 Practice for General Techniques of Gas Chromatography Infrared (GC/IR) Analysis²

3. Terminology

3.1 **Definitions**—For definitions of terms and symbols, refer to Terminology E 131.

4. Significance and Use

4.1 Infrared spectroscopy is the most widely used technique for identifying organic and inorganic materials. This practice

describes methods for the proper application of infrared spectroscopy.

5. General

5.1 Infrared (IR) qualitative analysis is carried out by functional group identification **(1-3)**³ or by the comparison of IR absorption spectra of unknown materials with those of known reference materials, or both. These spectra are obtained **(4-8)** through transmission, reflection, and other techniques, such as photoacoustic spectroscopy (PAS). Spectra that are to be compared should be obtained by the same technique and under the same conditions. Users of published reference spectra **(9-16)** should be aware that not all of these spectra are fully validated.

5.1.1 Instrumentation and accessories for infrared qualitative analysis are commercially available. The manufacturer's manual should be followed to ensure optimum performance and safety.

5.2 Transmission spectra are obtained by placing a thin uniform layer of the sample perpendicular to the infrared radiation path (see 9.5.1 for exception in order to eliminate interference fringes for thin films). The sample thickness must be adequate to cause a decrease in the radiant power reaching the detector at the absorption frequencies used in the analysis. For best results, the absorbance of the strongest bands should be in the range from 1 to 2, and several bands should have absorbances of 0.6 units or more. There are exceptions to this generalization based on the polarity of the molecules being measured. For example, saturated hydrocarbons are nonpolar, and their identifying bands are not strong enough unless the C-H stretch at 2920 cm⁻¹ is opaque and the deformation bands are in the range from 1.5 to 2.0 absorbance units (A) at 1440 to 1460 cm⁻¹. Spectra with different amounts of sample in the radiation path may be required to permit reliable analysis. If spectra are to be identified by computerized curve matching, the absorbance of the strongest band should be less than 1; otherwise, the effect of the instrument line shape function will cause errors in the relative intensities of bands in spectra measured by dispersive spectrometers and by FT-IR spectrometers with certain apodization functions (specially triangular).

5.2.1 Techniques for obtaining transmission spectra vary

¹ This practice is under the jurisdiction of ASTM Committee E-13 on Molecular Spectroscopy and is the direct responsibility of Subcommittee E13.03 on Infrared Spectroscopy.

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² *Annual Book of ASTM Standards*, Vol 03.06.

³ The boldface numbers in parentheses refer to a list of references at the end of the text.