



Standard Guide for Use of Spectral Searching by Curve Matching Algorithms with Data Recorded Using Mid-infrared Spectroscopy¹

This standard is issued under the fixed designation E 2310; 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 Spectral searching is the process whereby a spectrum of an unknown material is evaluated against a library (database) of digitally recorded reference spectra. The purpose of this evaluation is classification of the unknown and, where possible, identification of the unknown. Spectral searching is intended as a screening method to assist the analyst and is not an absolute identification technique. Spectral searching is not intended to replace an expert in infrared spectroscopy. Spectral searching should not be used without suitable training.

1.2 The user of this document should be aware that the results of a spectral search can be affected by the following factors described in Section 5: (1) Baselines, (2) sample purity, (3) Absorbance linearity (Beer's Law), (4) sample thickness, (5) sample technique and preparation, (6) physical state of the sample, (7) wavenumber range, (8) spectral resolution, and (9) choice of algorithm.

1.2.1 Many other factors can affect spectral searching results.

1.3 The scope of this document is to provide a guide for the use of search algorithms for mid-infrared spectroscopy. The methods described herein may be applicable to the use of these algorithms for other types of spectroscopic data, but each type of data search should be assessed separately.

1.4 The Euclidean distance algorithm and the first derivative Euclidean distance algorithm are described and their use discussed. The theory and common assumptions made when using search algorithms are also discussed, along with guidelines for the use and interpretation of the search results.

2. Referenced Documents

2.1 ASTM Standards:²

E 131 Terminology Relating to Molecular Spectroscopy

E 334 Practice for General Techniques of Infrared Microanalysis

E 573 Practices for Internal Reflectance Spectroscopy

E 1252 Practice for General Techniques of Qualitative Infrared Analysis

E 1642 Practice for General Techniques of Gas Chromatography Infrared (GC/IR) Analysis

E 2105 Practice for General Techniques of Thermogravimetric Analysis (TGA) Coupled with Infrared Analysis (TGA/IR)

E 2106 Practice for General Techniques of Liquid Chromatography—Infrared (LC/IR) and Size Exclusion Chromatography—Infrared (SEC/IR)

3. Terminology

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

3.1.1 *reference spectrum*—an established spectrum of a known compound or chemical sample.

3.1.1.1 *Discussion*—This spectrum is typically stored in retrievable format so that it may be compared against the sample spectrum of an analyte.

3.1.1.2 *Discussion*—This term has sometimes been used to refer to a background spectrum; such usage is not recommended.

3.1.2 *spectral searching*—the process whereby a spectrum of an unknown material is evaluated against a library of digital reference spectra. Each reference spectrum in the library is individually compared to the spectrum of the unknown, and assigned a numerical value as to the goodness of fit. To perform this comparison, each data point in the unknown spectrum is compared to each corresponding point in the reference spectrum.

3.1.3 *peak searching*—the process whereby the peak table of the spectrum of an unknown material is evaluated against a library of peak tables. Each reference spectrum in the library contains a peak table and the peak table is individually compared to the peak table of the unknown, and assigned a numerical value as to the goodness of fit.

3.1.4 *spectral library*—a collection of reference spectra stored in a computer readable form, also called a library, database, or spectral database.

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

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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.

