



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

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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 guide 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 guide 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.

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

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2. Referenced Documents

2.1 ASTM Standards:²

E131 Terminology Relating to Molecular Spectroscopy

E334 Practice for General Techniques of Infrared Microanalysis

E573 Practices for Internal Reflection Spectroscopy

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

E1642 Practice for General Techniques of Gas Chromatography Infrared (GC/IR) Analysis

E2105 Practice for General Techniques of Thermogravimetric Analysis (TGA) Coupled With Infrared Analysis (TGA/IR)

E2106 Practice for General Techniques of Liquid Chromatography-Infrared (LC/IR) and Size Exclusion Chromatography-Infrared (SEC/IR) Analyses

3. Terminology

3.1 *Definitions*—For general definitions of terms and symbols, refer to Terminology E131.

3.1.1 *Euclidean distance algorithm*—the Euclidean distance algorithm measures the Euclidean distance between each library spectrum and the unknown spectrum by treating the spectra as normalized vectors. The closeness of the match, or hit quality index (HQI), is calculated from the square root of the sum of the squares of the difference between the vectors for the unknown spectrum and each library spectrum.

3.1.2 *first derivative Euclidean distance algorithm*—in the first derivative Euclidean distance algorithm the Euclidean distance is also computed, except the derivative of each spectrum is calculated prior to the Euclidean distance calculation.

3.1.3 *hit quality index (HQI)*—a table which ranks the library spectra in the database according to their hit quality values (see 7.5).

3.1.4 *hit quality value*—the spectral search software compares each spectrum in the database to that of the unknown and

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.