



Designation: E 204 – 98

## Standard Practices for Identification of Material by Infrared Absorption Spectroscopy, Using the ASTM Coded Band and Chemical Classification Index<sup>1</sup>

This standard is issued under the fixed designation E 204; 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 ( $\epsilon$ ) indicates an editorial change since the last revision or reapproval.

### 1. Scope

1.1 These practices describe a data system generated from 1955 through 1974. It is in world-wide use as the largest publicly available data base. It is recognized that it does not represent the optimum way to generate a new data base with the most modern computerized equipment.

1.2 These practices describe procedures for identification of individual chemical substances using infrared absorption spectroscopy and band indexes of spectral data. Use of absorption spectroscopy for qualitative analysis has been described by many **(1-8)**,<sup>2</sup> but the rapid matching of the spectrogram of a sample with a spectral data in the literature by use of a band index system designed for machine sorting was contributed by Kuentzel **(9)**. It is on Kuentzel's system that the ASTM indexes of absorption spectral data are based.

1.3 Use of these practices requires, in addition to a recording spectrometer and access to published reference spectra, the encoded data and suitable data handling equipment.<sup>3</sup>

1.4 *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:

E 168 Practices for General Techniques of Infrared Quantitative Analysis<sup>4</sup>

E 932 Practice for Describing and Measuring Performance of Dispersive Infrared Spectrometers<sup>4</sup>

E 1252 Practice for General Techniques for Qualitative Infrared Analysis<sup>4</sup>

### 3. Summary of Practices

3.1 A representative sample of the material to be analyzed is separated into its individual components, if required, and each component is introduced into a suitable sample cell or matrix, mainly according to its physical state. The spectrum is recorded over a characterizing range. The choice of spectral range and instrument is dictated by a general consideration of the chemical nature of the sample **(3-5)**. A note is made of the spectral positions of prominent absorption bands and, optionally, of known chemical and physical properties of the material. The qualitative chemical composition of the material may then be identified by searching the coded data file for compounds having matching characteristics. Details on searching procedures are available elsewhere.<sup>5</sup> Details of the code are in the following sections.

### 4. Apparatus

4.1 *Infrared Spectrophotometer*—A spectrophotometer with capabilities equivalent to an instrument with a rock salt prism operated under parameters compatible with Analytical Spectra **(8, 10)** and with wavelength accuracy to 0.05  $\mu\text{m}$  by comparison with the indene spectrum in Practice E 932.

4.2 Laboratory procedures for obtaining spectra are described in Refs **(3-5)** and in Practices E 168, and E 1252.

4.3 *Data-Handling Equipment*—It is possible to convert data on the ASTM magnetic tape to IBM cards, and to use sorters or collators to manipulate the data. However, the file is large and it is more efficient, and with good software, more effective, to use computers. These may be either dedicated or time-shared. Thus, the minimum equipment requirement is a

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<sup>2</sup> The boldface numbers in parentheses refer to the list of references at the end of these practices.

<sup>3</sup> The *ASTM Infrared Spectral Index*, AMD 33 and its supplements may be purchased in the form of magnetic tapes, from Sadtler Research Labs., Inc., 3316 Spring Garden St., Philadelphia, PA 19104.

<sup>4</sup> *Annual Book of ASTM Standards*, Vol 03.06.

<sup>5</sup> Publicly available systems are as follows: *IRGO*, Chemir Labs., 761 W. Kirkham, St. Louis, MO 63122; *SPIR* (Canada only), National Research Council, 100 Sussex Dr., Ottawa, Ontario, Canada K1A 0R6.