



Designation: E204 – 98 (Reapproved2007)

# 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 E204; 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 cover 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:<sup>4</sup>

<sup>1</sup> These practices are under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Separation Science and are the direct responsibility of Subcommittee E13.03 on Infrared and Near Infrared Spectroscopy.

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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> 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.

[E168 Practices for General Techniques of Infrared Quantitative Analysis](#)

[E932 Practice for Describing and Measuring Performance of Dispersive Infrared Spectrometers](#)

[E1252 Practice for General Techniques for Obtaining Infrared Spectra for Qualitative Analysis](#)

## 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 E932.

4.2 Laboratory procedures for obtaining spectra are described in Refs (3-5) and in Practices E168, and E1252.

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

<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.

time-shared. Thus, the minimum equipment requirement is a computer, a program, and the coded data (and either batch processing facilities) or a teletypewriter or terminal with modem for accessing these resources<sup>5</sup> for interactive searches.

## 5. Index

5.1 The index data on approximately 145 000 spectra are available on magnetic tape. The main absorption bands of each spectrum are coded to the nearest 0.1  $\mu\text{m}$ .

5.2 In addition to the code for spectral data of chemical substances, there are codes for chemical-structure classification, empirical formula, melting or boiling point, and serial number reference. Other codes include data on sample state, wavelength intervals of strongest bands, and no-data areas. For a given substance, the coded spectral data are almost invariably unique as is the pattern for coded chemical structure and physical properties. Variables may be searched in any desired combination to locate a standard spectrum similar to that of a sample of unknown composition, to correlate type of structure with absorption band positions, to locate spectra of compounds having given structural features in common, and in other ways that are too numerous to include here.

5.3 Spectral and chemical data from the user's own laboratory may be coded in a compatible system from details given in subsequent sections.

5.4 Molecular formula-name tabulations comprise complementary data systems for use in conjunction with the spectral band codes and chemical classification tapes. These carry the molecular formulas, chemical names, and reference serial numbers for the compounds included in the indexes described in 5.1 and 5.2. The tapes are commercially available and the indexes have been published in book form as alphabetical, numerical, and molecular formula indexes (11,12,13). These books enable one to determine the name of the compound involved from a knowledge of the serial number of a spectrogram or to locate a published standard spectrogram for a compound when the name is known. The serial-number listing permits one to obtain the names of possible solutions to analytical problems from spectra serial numbers produced by search operations even though complete files of standard spectra (as listed in Table 1) are not at hand. Often the name of the compound together with other available information will suffice; however, it is desirable to have as many standard spectra as feasible on hand for detailed study and comparison, because positive identification depends upon matching the unknown spectrum with one from published material or one obtained from a *bona fide* sample of the compound. The molecular formula and alphabetical indexes are useful for accessing band data for a suspected answer to an unknown.

## 6. General

6.1 The system described below is designed to handle the spectral absorption data obtained in the spectral range from 2 to 16  $\mu\text{m}$ , and the system provides for a band-position coding resolution of 0.1  $\mu\text{m}$ .

6.2 The original coding was on an IBM card format. The numerical values therefore correspond to columns and rows. See Fig. 1.

**TABLE 1 Catalogs of Spectrograms Covered by ASTM Punched Cards Indexing Infrared Absorption Data**

A	API Research Project 44 <sup>A</sup>
B	User's own file of spectrograms <sup>B</sup>
C	Sadtler catalog of spectrograms <sup>C</sup>
D	NRC-NBS file of spectrograms <sup>D</sup>
E	Literature
F	Documentation of Molecular Spectroscopy <sup>E</sup>
G	Coblentz Society Spectrograms <sup>F</sup>
H	Chemical Manufacturer's Association (CMA) <sup>G</sup>
J	Infrared Data Committee of Japan <sup>H</sup>
K	Aldrich Library of Infrared Spectra <sup>I</sup> , 1970 Edition

<sup>A</sup> American Petroleum Institute, Research Project 44, *Infrared and Ultraviolet Spectral Data*, Texas Agricultural and Mechanical College, College Station, TX, 1943 to date. Loose-leaf.

<sup>B</sup> Users are encouraged to submit spectrograms (or the pure compound in some cases) to one of the other organizations listed. It is unlikely that any individual laboratory can code its spectral data and punch cards at the cost of the ASTM cards (about one cent each).

<sup>C</sup> *Standard and Commercial Spectra*, Sadtler Research Laboratories, 3316 Spring Garden St., Philadelphia, Pa. 19104. Loose-leaf. The Sadtler organization also offers a "Spec-Finder" book method of matching spectrograms with those in its catalog.

<sup>D</sup> *National Research Council-NBS Committee on Spectral Absorption Data*, National Bureau of Standards, Washington, D. C. 20025. Card file.

<sup>E</sup> *The DMS System*, Butterworth Scientific Publications, London WC2. Distributed in U. S. by Butterworth, Inc., 7235 Wisconsin Ave., Washington, D. C. 20014.

<sup>F</sup> *Coblentz Society Spectra*, sold by Sadtler Research Laboratories, 3316 Spring Garden St., Philadelphia, Pa. 19104 and The Coblentz Society, Inc., P.O. Box 9952, Kirkwood, MO 63122.

<sup>G</sup> Chemical Manufacturer's Association (CMA) 1825 Connecticut Ave., N. W., Washington, D. C. Loose-leaf. Spectra are no longer available from CMA.

<sup>H</sup> Infrared Data Committee of Japan, Sanyo Shuppan Doeki Co., Inc., Hoyo Bldg., 8, 2-chrome, Takaracho, Chuo-ku, Tokyo, Japan. Card file distributed in U. S. by Preston Technical Abstracts Co., 1718 Sherman Ave., Evanston, Ill.

<sup>I</sup> The Aldrich Library of Infrared Spectra, Aldrich Chemical Co., 940 N. St. Paul St., Milwaukee, Wis. 53233.

6.3 Columns 1 through 15 are used for coding absorption band positions.

6.4 The chemical classification code is in columns 32 through 57, and columns 58 through 62 provide for coding the number of C, N, O, and S atoms in the compound under consideration. A melting or boiling point is coded in 63 to 65. The rest of the card provides space for the private use of individual laboratories and the identification of the source of the coded data. The codes concerned with each of these areas are discussed separately.

## CODING OF INFRARED ABSORPTION BANDS (COLUMNS 1 THROUGH 25)

### 7. Codes for Absorption Band Positions

7.1 *Columns 1 to 15 of "A" Cards* (Note)—Coding is done in terms of wavelength in micrometres. From columns 1 through 15, the column number is taken as the whole number value of the absorption band, and the fractional part is rounded to the nearest 0.1  $\mu\text{m}$  (values ending in five hundredths are considered as next higher tenths) and the number corresponding to the 0.1  $\mu\text{m}$  value is added to the number of the column. Thus a band at 7.38  $\mu\text{m}$  is coded to correspond to position 4 in column 7, for a value of 7.4. The coding resolution of 0.1  $\mu\text{m}$  has been found to be adequate for searching and correlating published spectra.

NOTE 1—"A" is the designation for rock salt region infrared data (see 18.4).

