

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>

<sup>1</sup> These practices are under the jurisdiction of ASTM Committee E-13 on Molecular Spectroscopy and are the direct responsibility of Subcommittee E13.03on Infrared Spectroscopy.

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. 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 µm 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

Current edition approved Dec. 10, 1998. Published August 1999. Originally published as E 204–62T. Discontinued 1998. Reinstated December 1998.

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

<sup>&</sup>lt;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>&</sup>lt;sup>4</sup> Annual Book of ASTM Standards, Vol 03.06.

<sup>&</sup>lt;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 OR6.



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  $0.1 \mu m$ .
- 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  $\mu$ m, and the system provides for a band-position coding resolution of 0.1  $\mu$ m.
- 6.2 The original coding was on an IBM card format. The numerical values therefore correspond to columns and rows. See Fig. 1.
- 6.3 Columns 1 through 15 are used for coding absorption band positions.

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

	aoming a
Α	API Research Project 44 <sup>A</sup>
В	User's own file of spectrograms <sup>B</sup>
С	Sadtler catalog of spectrograms <sup>C</sup>
D	NRC-NBS file of spectrograms <sup>D</sup>
Ε	Literature
F	Documentation of Molecular Spectroscopy <sup>E</sup>
G	Coblentz Society Spectrograms <sup>F</sup>
Н	Chemical Manufacturer's Association (CMA) <sup>G</sup>
J	Infrared Data Committee of Japan <sup>H</sup>
K	Aldrich Library of Infrared Spectra <sup>1</sup> , 1970 Edition

<sup>&</sup>lt;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>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., Hoyu Bldg., 8, 2-chrome, Takaracho, Chuo-ku, Tokyo, Japan. Card file distributed in U. S. by Preston Technical Abstracts Co., 1718 Sherman Ave., Evanston, III.

<sup>1</sup>The Aldrich Library of Infrared Spectra, Aldrich Chemical Co., 940 N. St. Paul St., Milwaukee, Wis. 53233.

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  $\mu$ m (values ending in five hundredths are considered as next higher tenths) and the number corresponding to the 0.1  $\mu$ m value is added to the number of the column. Thus a band at 7.38  $\mu$ m is coded to correspond to position 4 in column 7, for a value of 7.4. The coding resolution of 0.1  $\mu$ 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).

7.2 Columns 1 to 25 of "G" for Far-Infrared—The coding of far-infrared absorption bands is done in terms of wavelength in micrometres. The whole number value of the band position

<sup>&</sup>lt;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>&</sup>lt;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.

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FIG. 1 Infrared Spectral Data Card

is obtained by adding 10 to the column number and the nearest tenth of a micrometre is represented by the decimal value to the nearest tenth. Thus, a band at  $18.57~\mu m$  is coded as 8.6.

7.3 To indicate the range of data covered by the spectrogram, an "x" code is coded for each column that codes a spectral range where no data are available. This is to distinguish such regions from those in the spectrogram that have been examined and found to contain no bands of sufficient intensity to code, or to mark those regions where the spectral data are obscured by strong solvent bands. Additionally, a "y" code is added to each column that indexes a very strong band. The coding of such strong bands is limited to a very few, usually about three, which may be expected to persist in the spectrum of a considerably diluted sample of the material. Use of such codes may be made in the analysis of mixtures where individual components may be present in relatively low concentrations so that only the strongest bands are readily detectable.

#### 8. Criteria for the Selection of Bands to be Coded

8.1 Experience has shown that it is not desirable to code all of the bands of most spectra. Major and medium strength bands are coded to identify the compounds uniquely. However, coding of too many weak bands minimizes the effectiveness of negative searching, which is valuable for mixtures. Therefore, the selection of which bands to code and which to omit requires some judgment; and because of the nature of published spectrograms, the judging can be guided only by rather flexible rules. Several factors enter into the determination of the strength of an absorption band, and what may be a good set of factors for the production of an excellent spectrogram from one material is not necessarily a good set to provide a spectrogram from another material. Moreover, the quality of published spectra varies widely and any system of coding absorption bands must allow for making the best possible use of all such data.

8.2 As a general rule, bands selected to be coded have an absorbance ratio with the strongest band in the spectrogram of 1:10 or more. This means that when the strongest band has between 1 and 5 % transmittance, bands are coded which have 70 % or less transmittance as measured from a reasonably

adjacent background (not necessarily at 100 % transmittance); or if the strongest band is between 5 and 20 % transmittance, bands are coded which have 80 % or less transmittance as measured from a reasonably adjacent background. Thus, to be coded, a band stands out from its adjacent background, at least on one side, by 20 to 30 % transmittance on the chart. Therefore, "shoulders" and weak bands on the sides of strong bands are not coded. Likewise, bands whose percent transmittance may be as low as 60 to 50 as read from the chart, but which extend from backgrounds having transmittance values of 80 to 70 %, are not coded. Some examples are provided in Fig.

8.3 Searching absorption band data is much the same as coding the bands. First, the spectrogram of the unknown material should have its strongest bands between 1 and 20 % transmittance since it is to be compared with data coded on that basis. Then one proceeds by two different methods depending upon whether the unknown is a single component or is a mixture of two or more components in roughly equivalent amounts. In the former case, positive searching on the bands is in order, while the latter case requires that negative inputs be included in the search request. Each method is discussed briefly in Sections 9 and 10.

8.4 The optimum combination of searching techniques depends upon the computer algorithm used. Instructions specific for each program should be followed.<sup>5</sup>

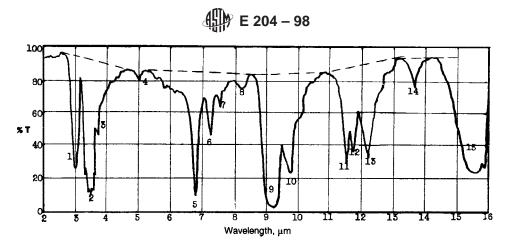
#### 9. Positive Searching for Individual Spectra

9.1 In this method, the search data are selected with the expectation that all or most of the bands in the unknown spectrogram are caused by a single compound. Search programs vary, but it is desirable that they include provisions for weighting the bands by their importance. This weighting may be systematic, as by the strength of the bands, or it may be on the basis of bands that the spectroscopist recognizes as important for other reasons.

9.2 If one cannot be certain to 0.1  $\mu m$  of the location of the band, then searching should be carried out over as broad an interval as required to make certain the band is included in the search. Thus, a particular band on the original standard spectrogram may have been measured to be 13.46  $\mu m$ . When it

NOTICE: This standard has either been superceded and replaced by a new version or discontinued.

Contact ASTM International (www.astm.org) for the latest information.



Note 1—The above hypothetical spectrogram is included to assist in describing the application of rules prescribing which bands to code and which to omit from the index card. It will be noted that band No. 9 is the strongest and has a transmittance value between 1 and 5 %; therefore all bands having a transmittance of 70 % or less as measured against a reasonably adjacent background should be coded. The dotted lines indicate what is meant by such an adjacent background. The distance by which coded bands must project from such a background is equal to one and a half units of the vertical scale. Applying this rule, one can code without question the following bands: No. 1, 2, 5, 6, 9, 10, 11, 12, 13, and 15, and furthermore, bands 2, 9 and 15 should receive the "y" overpunch code also. Band No. 5, while rather strong, is not expected to persist in considerably diluted samples of this material.

It will be noted that band No. 3 was not included. This is a case of a rather weak band on the side of a strong one which has no value in sorting and need not clutter up the card. Therefore it was omitted. On the other hand, band No. 10 was included as it is prominent enough to be used in sorting operations. Also, No. 12, which does not fit the coding criteria when measured from its immediately adjacent background, is included in those bands coded because it obviously is one of three rather strong bands which are close enough together to overlap appreciably. An ill-defined shoulder on the side of band No. 10 is ignored as is the fine structure in the No. 2 band. Band No. 14 represents a possible borderline case that should not be coded. A good rule is "when in doubt, leave it out." The spectrogram is typical of many that appear published in the literature and serves to illustrate why a coding resolution of 0.1 µm is entirely adequate.

#### FIG. 2 Example of Infrared Curve

was coded the position was 13.5, or number 5 in column 13. In an unknown spectrogram, this same band might be read as 13.44, or if a longer cell path was used the band may have spread to the extent that one cannot be certain whether the minimum is 13.4 or 13.5  $\mu$ m. In such a case, the search program should accept 13.4 or 13.5  $\mu$ m, or both, and thus not miss the desired compound.

#### 10. Negative Searching for the Analysis of Mixtures

10.1 When the unknown infrared spectrogram represents a mixture of two or more compounds in appreciable amounts, positive searching on the absorption band positions must

follow a procedure that considers the many possible combinations of bands that may characterize an individual constituent, since it is not known which bands are produced by each component. Such an approach may be carried out directly on the spectrogram of a mixture. However, considerable time may be saved if the bands are subjected to "negative" searching to eliminate all of the spectra that do have bands in regions of the spectrum where the unknown spectrogram does not have bands, since none of these could possibly be a component of the mixture. Positive searching of the reduced spectral file which results from the negative searching is more selective than searching the total file.



TABLE 2 Chemical Classification Code Chart Part A

			Fait A				
Row	Column 32 Elements	Column 34 Structure	Rov	N	Column 36 Code Units	Column 38 Miscellaneous	Row
0	0	acyclic	0		12 or more	solid	0
1	N	alicyclic	1		1	liquid	1
2	S F	aromatic	2		2 3	gas	2
3 4	Cl	heterocyclic fused alicyclic	3		4	organo-metallic isotopic	4
5	Br, I	fused ancyclic	5		5	indeterminate	5
6	P, Bi	fused heterocyclic			6	solution	6
7	As, Sb	racea neterecyone	7		7	polymer	7
8	Si, Ge	3 or 4-member rin			8	chelate	8
9	Sn, Pb	5-member ring	9		9	hydrate	9
X	B, Al	6-member ring	X		10	salt plate	X
Υ	other	7-or more member	r ring Y		11	•	Υ
Row	Column 33 Unsaturation	Column 35 Rings—Chains	ſ	Row	Column 37 Substitutions	Column 39 Miscellaneous	Row
0	ring	rings		0	[mono]	cis	0
1	1	1		1	1 [1, 2]	trans	1
2	2	2		2	2 [1, 3]	spiro	2
3	3	3		3	3 [1, 4]	dextrorotary	3
4	4	4		4	4 [1, 2, 3]	levorotary	4
5	5	5		5	5 [1, 2, 4]	symmetrical	5
6	6	6		6	6 [1, 3, 5]	unsymmetrical	6
7	7	7		7	7 [1, 2, 3, 4]	vicinal	7
8	8	8		8	8 [1, 2, 4, 5]	salt	8
9 X	9	9		X	9 [1, 2, 3, 5] 10 [penta]	inorganic ester	9 X
^	C <u></u> C	10		Mual	10 [penta]		^
Υ	—C≡C—	11 or more	/stand	Y	[hexa]	inorganic	Υ
			Part B				
_	Column 40	Column 42	Column 44	4 Drea	Column	n 46 Column 48	_
Row	C—H	0		Row	VIEW s	N—O	Row
						>NC( = 0)0—	
			İ			>NO( — 0)0—	
			C(N)N<			OC(=-N)O	
0	—CH <sub>3</sub> methyl	-C(=O)OH	TROTTVILL	0	-c(=s)s		0
	ps://standards.iteh.ai/ca	atalog/standard			e7d-ae2d-b72	3470 > NC(=0)N<	-e204 <sup>0</sup> 98
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			>NC(=:\bar{N})N<			—OC( <b>≕</b> N)N<	
1	—C <sub>2</sub> H <sub>5</sub> ethyl	-C(=0)0-	, ,	1	-C(=S)H	,	1
	2 3 ,	,			,	-C(=O)N<	
						ì	
						—C( <u>—</u> N)O—	
2	—C₃H <sub>7</sub> n-propyl	-C(=O)H	—CN	2	>C = S		2
3	—C₃H <sub>7</sub> isopropyl	>C = O	-NC	3	-SC(=S)S	S— —NCO	3
4	—C₄H <sub>9</sub> <i>n</i> -butyl	-00(=0)0-	-NH <sub>2</sub>	4	—SH `	—OCN	4
5	—C₄H <sub>9</sub> isobutyl	$C(OR)_4$ — $C(OR)_3$	>NH	5	—S—	>NNO <sub>2</sub>	5
6	—C₄H <sub>9</sub> sec-butyl	$-C(OR)_3$	>N—	6	—SS—	>NNO	6
7	—C₄H <sub>9</sub> terbutyl	—OH	>C = N-	7	>S <sup>+</sup>	-NN(=O)-	7
0	0.11	0	= NN =	2	<b>— 0</b> 0	ONO	0
8	—C₅H₁₁n-pentyl	-0-	>NN< —N = N—	8	= S = S	-ONO <sub>2</sub>	8
9	—C <sub>6</sub> H <sub>5</sub> phenyl	-00-	—N — N— — N≡N	9		-on = o	9
X	061 15 PHOLIST	other	other	X	other	other	X
Ϋ́		heterocyclic	heterocyclic	Ŷ	heterocyclic	heterocyclic	Ŷ
	Column 41	Column 43	Column 45		Column		
Row	C—H	0	N	Row	S	N—O	Row
0	$-CH = CH_2 \text{ vinyl}$	>0+	_N = N_N<	0		-NO <sub>2</sub>	0
1	$>C = CH_2 termethylene$	-O <sub>3</sub>	$-N = N^+$	1		—NO <sub>2</sub> —NO	1
2	= CHCH <sub>3</sub> ethylidene	>C(—O—) <sub>2</sub>	-N+	2		= NO-	2
-	or for is outly induffe	- 12	•	_		> NO—	_
3	-CH2CH = CH2 allyl		-NH <sub>4</sub>	3		>N = 0	3
4	—CH = CHCH <sub>3</sub> propenyl		>NCN	4		-	4
5	$-C(CH_3) = CH_2$ isopropenyl		-N <sub>3</sub>	5			5
6	= C(CH <sub>3</sub> ) <sub>2</sub> isopropylidine		Ü	6			6
7	—C≡CH ethynyl			7			7
8	—C≡CCH <sub>3</sub> 1-propynyl			8			8



Part	В
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Row	Column 40 C—H	Column 42 O	Column 44 N	Row	Column 46 S	Column 48 N—O	Row
9	—CH <sub>2</sub> C≡CH 2-propynyl			9			9
X	conjugated	conjugated	conjugated	X co	onjugated	conjugated	X
Υ	, 0	, 0	, 0	Υ	, 0	, 0	Υ
Row	Column 50 N—	Column 52 O—S	Row	Column N—O—		lumn 56 ements	Row
0	>NC( = S)N<	-OC(= S)S $-$	0	>NC(= S)O-	Se, Te,	Po	0
	-SC(=N)N<	-sc(=o)s-		>NC(=0)S-			
1	>NC(=S)S-	-00(=5)0-	1	-C(=O)NS-	- Ga, In, <sup>-</sup>	TI	1
	-SC(=N)S-	-OC(=O)S-		-C(=S)NO-	-		
2	-C(=S)N<	-c(=s)o-	2	-OC(=N)S-	- Zn, Cd,	Hg	2
	-C(=N)S-	-C(=O)S-				-	
3		-S(O <sub>2</sub> )O-	3	-S(=O)N<	Cu, Ag,	Au	3
4	—SCN	-s(=0)0-	4	>NS(O <sub>2</sub> )N<	Fe, Co,	Ni, Mn	4
5	-NCS	-s(=o)s-	5	>NS(O <sub>2</sub> )O—	Cr, Mo,	W, U	5
		-s(=s)o-					
6	>NSN<	S <sub>x</sub> O <sub>6</sub>	6	>NS(O <sub>2</sub> )—	V, Cb, T	a, Pa	6
		(x = 2-6)					
7	= NS $-$	>SO <sub>2</sub>	7	>NS(=O)O-	Ti, Zr, H	f, Th	7
	> NS						
8	-N = S	> S = 0	8	-NSO	Se, Y, L	a, Ac	8
9	>S = N-	-OSO-	9		Ru, Rh,	Pd, Os, Ir,	9
					Pt		
X	other	other	X	other	rare ear	ths	X
Υ	heterocyclic	heterocyclic	Υ	heterocyclic	heterocy	/clic	Υ

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