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COBLENTZ SOCIETY SPECTRAL EVALUATION COMMITTEE†

**SPECIFICATIONS FOR INFRARED
REFERENCE SPECTRA OF MOLECULES
IN THE VAPOR PHASE**

(Recommendations 1987)

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Specifications for infrared reference spectra of molecules in the vapor phase (Recommendations 1987)

Abstract - The document supplies specifications for the measurement, collection, presentation and storage of high quality infrared reference spectra of materials in the vapor phase. The specifications include details of instrument conditions to be used, sampling procedures, hard copy presentation of data, classification of data to facilitate later spectral searching, and recommendations for digital storage. A summary of the parameters for storing spectra on magnetic tape is also presented.

PREAMBLE

Introduction

Infrared spectrometry is being used to an increasing extent for the qualitative and quantitative analysis of trace components of the atmosphere. Several collections of reference spectra of samples in the vapor phase at ambient temperature are now available (1-6). The spectra in these collections are measured at medium resolution ($\Delta\tilde{\nu} = 1 - 4 \text{ cm}^{-1}$); in some the samples are neat at low pressure while in others an atmosphere of air or nitrogen has been added. Although these reference data are certainly useful to the many users of medium resolution spectrometers (both grating and Fourier transform), the spectra have been measured at too high resolution to provide even semi-quantitative calibration factors for users of tunable diode laser (TDL) spectrometers. There is now a very definite need for collections of spectra of samples in the vapor phase, measured at a variety of resolutions, with and without air broadening, in as uniform a format as possible.

Many infrared spectrometers are now mini- and micro-computer controlled, and can readily generate data in digital form for archival storage. In order for digitally stored data to be readily transferable from one site to another, it is necessary to ensure that the format of the stored information is as uniform as possible. In this document we are not only proposing specifications for the measurement and presentation, as hard copy, of infrared reference spectra of molecules in the vapor phase, but also for formatting digitally stored reference data on magnetic tape.

Instrumental conditions

Unlike the criteria previously proposed by the Coblenz Society (7), and subsequently approved by the International Union of Pure and Applied Chemistry, for medium resolution reference spectra of condensed phase samples (8), equally firm specifications cannot be proposed which are rigidly applicable to the many different types of instruments used for measuring vapor phase spectra. For example, a reference spectrum measured using a selective wavelength analyzer is of little or no use to users of TDL spectrometers, and *vice versa*. Thus, we are proposing that reference spectra measured on any type of infrared spectrometer should not be rejected simply on the grounds of resolution, but rather that the resolution should be recorded with the data. In theory, at least, reference spectra measured at very high resolution may be degraded to simulate spectra measured on a lower resolution spectrometer by convolution of the high resolution spectrum with the instrument line shape function of the lower resolution spectrometer. Thus, primary emphasis should be placed on the acquisition of high resolution data ($\Delta\tilde{\nu} < 1 \text{ cm}^{-1}$), over as wide a spectral range as possible.

Spectra should be plotted over a "useful" wavenumber range, without extensive regions where little or no information on the sample of interest is present. For spectra measured at medium or low resolution ($\Delta\tilde{\nu} > 1 \text{ cm}^{-1}$), no regions of the spectrum should be left blank. For spectra measured at higher resolution, spectra should only be plotted in regions where "significant" spectral information is to be found. Obviously what is "significant" will vary from application to application and from laboratory to laboratory, but as a default condition we define "significant" information as an absorption band containing at least one feature with a peak absorbance greater than 0.05.

Specification of the low wavenumber cutoff also presents a problem. In many cases the lower wavenumber limit of spectrometers with KBr optics (400 cm^{-1}) may not be low enough to enable the lowest frequency fundamental modes of some heavy molecules to be measured. On the other hand, the increasingly popular use of the mercury cadmium telluride photodetector on many spectrometers may necessitate a cutoff as high as 700 cm^{-1} . Thus we have specified as an upper limit a low wavenumber cutoff for reference spectra as 700 cm^{-1} , with the recommendation that spectra be plotted to lower wavenumbers than this if possible.

Sampling

Ideally vapor phase spectra should be measured under at least two conditions, both neat at low pressure (self-broadening) and with an atmosphere of dry air free of CO₂ added (air-broadening). As an alternative to air, dry nitrogen can be added (nitrogen-broadening). The (partial) pressure of the sample should be great enough to cause the strongest features to absorb between about 70% and 90% of the incident radiation. If important weak bands are present, the spectra should be rerun at higher pressure or at longer pathlength to yield an interpretable spectrum in this region. Samples should be held at ambient temperature unless an increase in temperature is needed to prevent sample condensation in the cell.

Since quantitative data are required, an accurate knowledge of the pathlength of the cell and (partial) pressure of the sample is necessary. The product of these two parameters should be accurate to better than $\pm 10\%$. If the error limits are believed to lie outside this range, they should be estimated and recorded.

Presentation of data

Spectra should be plotted linearly in transmittance or percent transmission on charts which are linear in transmittance or percent transmission, since this is the format in which they are usually measured originally. Nonlinear absorbance grids are acceptable but not recommended. Spectra plotted linearly in absorbance are also acceptable but again not recommended.

Spectra are to be plotted with high wavenumber to the left, and in such a format as to permit clear identification of each feature. To this end, the abscissal scale expansion and pen width should provide a trace in which the width of the plotted line is at least four times narrower than the full width at half maximum absorbance of the narrowest spectral feature.

It is recognized that it is often difficult to prepare absolutely pure samples. If impurity bands are apparent on a reference spectrum, they should be indicated and preferably identified.

Classification of data

Since the spectra of vapor phase samples are so strongly dependent on instrumental resolution and the presence or absence of a broadening gas, spectral search routines using vapor phase reference spectra must be applied with great care. To simplify the programming for spectral search and to provide a simple classification for vapor phase reference data, we propose the following classification:

a. Instrumental Resolution: A number will be assigned to a spectrum to denote that the resolution of the instrument fell in a certain range. This number will change each time the resolution changes by a factor of $\sqrt{10}$, and will be equal to $2[1 - \log_{10}(R/\text{cm}^{-1})]$, where R is the minimum numerical resolution (cm^{-1}) in the range. The code will be as follows (Table 1):

Table 1

Numerical Code	Resolution (cm^{-1})	
	Greater than	Less than
0	10	30
1	3	10
2	1	3
3	0.3	1
4	0.1	0.3
5	0.03	0.1
6	0.01	0.03
7	0.003	0.01
8	0.001	0.003
9		0.001

b. Broadening Gas: A letter will be assigned to the spectrum to denote the nature of the broadening gas. This letter will immediately follow the numerical code above. The letter code will be as follows:

S	self-broadened;
A	broadened with one atmosphere of air, free of water and carbon dioxide;
N	broadened with one atmosphere of dry nitrogen;
X	broadened by some other gas.

Thus a reference spectrum of a gas broadened by nitrogen and measured at 2 cm^{-1} resolution will be given the classification of 2N. In this way it is a simple matter to program a search. If, for example, a spectrum of an unknown in air is measured at 4 cm^{-1} , it is probable that only reference spectra with the classification 1N, 1A, 2N and 2A would be searched initially. If no matching spectrum is found, it may also be desirable to subsequently search the 1S and 2S data base.

Digital storage

Perhaps the most universal medium for digital storage of data is magnetic tape. We are therefore proposing a format for data stored on magnetic tape and we hope that this format may be easily modified for data stored on other media, e.g. punched cards or discs. The format which we propose is similar to the format proposed earlier by another subcommittee for GC-IR reference data (8).

Digitally stored reference data must contain at least two sets of data, a general name and data file (file A) and the digitized spectrum itself (file B). The absorbance spectrum is used in preference to the transmittance spectrum since it is more closely related to the fundamental parameter, the absorption coefficient and within certain limitations line or band intensities are directly proportional to the (partial) pressure of the sample.

The wavenumber interval at which spectra are digitized is a matter of some controversy. In theory, if the instrument line shape function (slit function) of the spectrometer is known and used as an interpolation function, only one data point per resolution element need be stored in order for the original analog spectrum to be completely reproduced. In practice, if at least two data points per resolution element have been sampled, many commonly used interpolation functions can be applied in order to accurately reproduce the analog trace of the spectrometer. As progressively smaller sampling intervals are used, the digital spectrum plotted using only linear interpolation more closely approximates the analog spectrum, but the storage required gets unnecessarily high. Therefore, the specification of at least two data points per resolution element and a known instrument line shape function has been adopted for all spectra measured on spectrometers other than TDL spectrometers. For laser spectrometers the half width of the laser line is considerably less than the Doppler width of each line in the spectrum. Therefore, in this case, we would recommend a minimum sampling interval of $1 \times 10^{-3}\text{ cm}^{-1}$ or one half the Doppler width, with a large interval for air-broadened spectra.

In an attempt to produce an efficient storage format, the data base will be stored in FORTRAN readable unformatted magnetic tape records (although File A may be considered formatted since the character data cannot be stored more efficiently in an unformatted mode). Since most computer systems can read IBM compatible formats, this format mode is considered the most convenient. Since the data records are unformatted, the use of ASCII Variable Block Size record formats is required. Some computer systems have low limits on the maximum record length, so the record length has been limited to 2058 8-bit bytes, the first eight bytes of which are header information bytes used by the tape handlers for assessing the actual record length. Thus, for a spectrum recorded from 4000 to 400 cm^{-1} with a sampling interval of exactly 2 cm^{-1} , there are 1801 data points which can be recorded in 3602 bytes. This results in two records, one 2050 ($2048 + 2$) bytes in length, and the other 1556 ($1554 + 2$) bytes. All records have two more bytes than required by the number of data points to allow the serial number of the spectrum to be written in the first two bytes of each record.

A typical schematic for a tape is shown in Fig. 1 of reference (9). The first two bytes are the total byte length of the physical record (including those two bytes). For file A of the digitally stored data described in the section on RECORDING ON MAGNETIC TAPE, File A - Information Record and Table 2, *vide infra*, the data length is 624_{10} bytes, plus eight bytes for the header. Thus the total record length is 632_{10} bytes which, expressed as a hexadecimal number, is 278_{16} . The next two bytes must be null, or zero. Bytes five and six are the logical record length, which, in this case, is the entire remainder of the record; i.e., 628_{10} bytes, or 274_{16} . Bytes seven and eight must also be null in this case. The header blocks for file B are generated in an analogous fashion. Employing the correct Job Control Language Statements, IBM systems will automatically write and read these header blocks; however, many other computer systems will not read them. To generate the header block for file A on such systems, eight should be added to the data record length, and that number expressed hexadecimally, should be written in the first 2-byte work of the record. A null word follows; i.e., a word of zeros, then the data record length plus four, another null word, and finally the data. Upon reading these records on non-IBM systems, the first eight bytes may simply be ignored.

SPECTROMETER OPERATION

Spectral range

For spectra measured at a resolution of 1 cm^{-1} or lower resolution ($\Delta\tilde{\nu} > 1\text{ cm}^{-1}$), spectra should be recorded from 4000 cm^{-1} to 700 cm^{-1} or below without gaps; reduction of the lower limit to 400 cm^{-1} is encouraged. For spectra measured at higher resolution ($\Delta\tilde{\nu} < 1\text{ cm}^{-1}$), spectral regions in which no absorption feature of the sample shows an absorbance greater than 0.05 need not be recorded. For very high resolution spectra ($\Delta\tilde{\nu} < 0.01\text{ cm}^{-1}$) reference spectra of single bands are acceptable.

Resolution

The resolution, given as the full width at half maximum of the instrument line shape function, should appear on the chart. No restrictions on the resolution are specified since reference spectra are needed at a variety of resolutions. Every effort, however, should be made to ensure that the instrumental resolution does not change dramatically across the spectrum.

Abscissa

The abscissal scale should be linear in wavenumber. Scale changes on low resolution spectra (e.g., a 2:1 scale change at 2000 cm^{-1}) are acceptable but not desirable. Spectra should be plotted from high to low wavenumber with high wavenumber to the left.

Wavenumber accuracy

The frequencies of sharp absorption features as read from the chart should be accurate to one half the resolution for all spectra except those measured using a laser spectrometer. The wavenumbers of spectra measured using a laser spectrometer should be accurate to $2 \times 10^{-3}\text{ cm}^{-1}$.

Noise level

The peak-to-peak noise level in the spectrum should not exceed 2% of full scale, except over very short regions where no absorption bands of the sample are observable (such as the 2347 cm^{-1} band due to carbon dioxide). It is preferable that digital smoothing routines are not applied to the spectra after acquisition except for the purpose of reducing the resolution of a reference spectrum in order to simulate data measured at a lower resolution on a different instrument. If a smoothing function is used, it must be specifically defined.

Ordinate expansion

If, for some reason, the absorbance of the strongest feature in the spectrum does not exceed 0.50, the spectrum may be measured or replotted using ordinate scale expansion (zero suppression), provided that the ratio of the peak absorbance of the strongest feature in the spectrum to the maximum peak-to-peak noise level in the spectrum is at least 40:1. When a spectrum is measured or plotted using ordinate expansion it must be clearly indicated on the chart, and the measured peak absorbance of the most intense spectral feature must be given.

Baseline flatness

The baseline (I_0 line, 100% line) must be flat to better than 5% of full scale across the recorded spectrum.

Recording

It is permissible for spectra to appear on more than one chart, even though for low or medium resolution spectra ($\Delta\tilde{\nu} > 1\text{ cm}^{-1}$) no spectral regions should be omitted. Discontinuities in the ordinate scale should not exceed 2%. Hand retraced spectra are unacceptable.

Atmospheric interferences

The effects of atmospheric water vapor lines should not exceed the allowable noise level (see SPECTROMETER OPERATION, Wavenumber Accuracy). The effect of CO_2 absorption lines can exceed this level provided that the sample has no absorption features around the 2347 or 668 cm^{-1} bands of CO_2 .

Ordinate scale

It is preferred that the intensity ordinate values be plotted linearly in transmittance or percent transmission on charts with a linear transmittance or percent transmission grid; a logarithmic ordinate grid or spectra plotted linearly in absorbance are acceptable. Note: This specification does not refer to digitally recorded data on magnetic tape, but only to the original hard-copy record.

Pen width

The width of the plotted line should be at least four times less than the resolution for all spectra other than those recorded using TDL spectrometers. For spectra measured using a laser spectrometer, the width of the plotted line should be at least four times less than the width of the narrowest absorption feature in the spectrum.

Apodization function

Spectra measured using a Fourier transform spectrometer should be computed from the interferogram using a triangular apodization function.

SAMPLE HANDLING**Peak absorbance**

All samples must be present in the cell so that the combination of partial pressure of the sample and pathlength of the cell causes the strongest feature in each plotted range to have a peak absorbance of between 1.0 and 0.50.

Pressure

Samples may either be present in the cell with no foreign gas present or, with an atmosphere of dry air (free of CO₂), nitrogen, or some other gas added. In all cases, the (partial) pressure of the sample and (where applicable) the partial pressure and identity of the added gas should be recorded on the chart.

Temperature

All spectra should be measured with the sample at ambient temperature, unless an increased temperature is needed to permit a sufficiently high sample vapor pressure for the peak absorbance criterion to be obeyed (see SPECTROMETER OPERATION, Ordinate Expansion and SAMPLING HANDLING, Peak Absorbance). The temperature should be recorded on the chart for all spectra.

Cell pathlength

No restriction is placed on the cell pathlength. The pathlength should be recorded on the chart for all spectra.

Quantitative accuracy

The product of the pathlength of the cell and the (partial) pressure of the sample should be accurate to better than $\pm 10\%$. If the error limits are believed to lie outside this range, the estimated limits should be recorded on the chart.

INFORMATION TO APPEAR WITH THE SPECTRUM (HARD COPY)**Sample**

Both the structural and the molecular formula should appear on the chart. It is also recommended that the compound name be included, and that the name should conform with the nomenclature used by IUPAC. Common or proprietary names and the CAS Registry Number can be included if desired. The source of the sample should also be included. The (partial) pressure of the sample (Pa) should be recorded along with the pressure and identity of the added gas (where applicable) and the temperature of the sample (K).

Instrumental

The make and model of the spectrometer should be recorded, as well as the date on which the spectrum was measured. For spectra measured on dispersive spectrometers, all changes of gratings and filters should be recorded, together with the wavenumber at which they occur and the slit program used. The resolution at which the spectrum was measured should be recorded, together with the alphanumeric classification (see PREAMBLE, Classification of Data).

Peak absorbance

The peak absorbance of the strongest band in the spectrum should be given. If a second spectral plot was necessary, the conditions under which the second spectrum was measured or plotted should appear on the chart. If ordinate expansion was required, an indication should also appear with the spectrum.

RECORDING ON MAGNETIC TAPE

General

For spectra measured on spectrophotometers with a digital data system, data should also be output on magnetic tape, both for archival purposes and for later modification to computer searchable files. The aim for magnetic tape storage should be to store data in a uniform manner no matter on what type of spectrometer or data system the spectra have been measured. To this end, it is recommended that data be written on 9-track magnetic tape at 800 bpi in FORTRAN readable, IBM compatible, unformatted records. Since the data records are unformatted the use of ASC11 Variable Block Size record formats is required. The record length will be limited to 2058 8-bit bytes (see PREAMBLE, Digital Storage).

Two files are required for each spectrum. File A will contain the sample information and instrument parameters. File B will contain the absorbance spectrum of the sample. Only a single spectrum will be stored in this file; spectra run under different conditions (e.g., sample pressure, air-broadening, resolution) will be stored in a separate file with a separate header. At least two points per resolution element will be stored for spectra measured at resolutions down to 0.003 cm^{-1} . For spectra measured at higher resolution, a sampling interval of 0.001 cm^{-1} is acceptable.

File A—information record

The information stored in file A concerns compound identification and properties, parameters for the spectrum stored in file B, sampling parameters, instrumental details, and contributor information. A schematic of the nature, format and degree of necessity for File A is shown in Table 2. It may be summarized as follows:

Field number 1 through 6: Compound identification and properties. These fields include a contributor-assigned serial number, molecular formula, connectivity matrix or Chemical Abstracts Service registry number, common and IUPAC or CAS name, and molecular weight. The connectivity matrix is one which describes the structure of the compound.

Field number 7 through 10: Parameters for the absorbance spectrum stored in file B. These fields include the starting and final wavenumber, sampling interval and number of data points. The starting wavenumber should always be greater than the final wavenumber.

Field number 11 through 14: Sampling information, such as sample pressure, broadening gas pressure, cell pathlength and temperature.

Field number 15 through 21: Instrumental information, such as the manufacturer and model number of the spectrometer, grating and filter changes and detector. The resolution is specified at three different wavenumbers (750 , 1500 and 3000 cm^{-1}), since the spectral resolution is not constant on many types of spectrometers.

Field number 22: Alphanumeric classification code for spectrum (see PREAMBLE, Classification of Data).

Field number 23 through 25: Contributor information, such as the date, and the operator's name and laboratory.

File B—absorbance spectrum

After the IBM header data, the first two bytes of each data record will contain an integral serial number corresponding to the serial number in field No. 1 of file A. Each spectrum will be divided up into records of 1024 data points (2048 bytes) as discussed in the PREAMBLE, Digital Storage. The final record of each spectrum may be shorter than 2048 bytes.

The ordinates will be expressed to 0.002 absorbance units from 0.000 to 1.998. In order to save space, the absorbance units will be expressed as integers (0 to 1998) by multiplying each ordinate by 1000.

Table 2. Information Record

Field No.	No. of bytes required	Description	Suggested Format	Degree of necessity
1	10	Serial number, contributor assigned	I10	Mandatory
2	32	Molecular formula <u>e.g.</u> , C.2.F.5.Cl.1	32A1	Mandatory
3	12	Connectivity matrix ^a and/or CAS Registry Number	12A1	Mandatory
4	128	Common or proprietary name(s), <u>e.g.</u> , FREON 115; use a semi-colon and a blank to separate each name.	128A1	Mandatory, if applicable
5	256	IUPAC name, <u>e.g.</u> , CHLOROPENTAFLUOROETHANE	256A1	Mandatory
6	7	Molecular weight	F7.2	Desirable
7	10	Starting spectrum wavenumber	F10.4	Mandatory
8	10	Final spectrum wavenumber	F10.4	Mandatory
9	8	Sampling interval, cm ⁻¹	F8.5	Mandatory
10	7	Number of spectrum points	I7	Mandatory
11	8	(Partial) pressure of sample, kPa (see footnote)	F8.5	Mandatory
12	4	Partial pressure of broadening gas kPa	I4	Mandatory
13	7	Cell length, mm	I7	Mandatory
14	6	Cell temperature, °C	F6.1	Mandatory
15	32	Manufacturer and model number of spectrometer	32A1	Mandatory
16	5	Nominal resolution at 750 cm ⁻¹ , cm ⁻¹	F5.3	Mandatory
17	5	Nominal resolution at 1500 cm ⁻¹ , cm ⁻¹	F5.3	Mandatory
18	5	Nominal resolution at 3000 cm ⁻¹ , cm ⁻¹	F5.3	Mandatory
19	32	Grating changes, cm ⁻¹	32A1	Desirable, if applicable
20	32	Filter changes, cm ⁻¹	32A1	Desirable, if applicable
21	32	Infrared detector type	32A1	Very desirable
22	2	Spectrum classification code from PREAMBLE, Classification of Data	2A1	Mandatory
23	32	Operator's name	32A1	Mandatory
24	10	Date spectrum was measured, Month-Date-Year, <u>e.g.</u> , 02-09-1981	10A1	Mandatory
25	32	Laboratory name	32A1	Mandatory

^aAny matrix that describes structural features and is transferable.

FUTURE NEEDS

To a certain extent this may be considered to be a preliminary document in that, whereas specifications as to, for example, the wavenumber accuracy and spectrometer resolution have been set down, no universally accepted method of testing these specifications has been found. For example, the wavenumber calibration data published in the two IUPAC-sponsored books (10,11) are sufficient for many users of fairly high resolution spectrometers but not good enough at all wavenumbers for users of laser spectrometers. If spectra are measured at lower resolution, lines begin to blend and shift and so these data once again cannot be used. Obtaining accurate, reliable data for wavenumber calibration across the complete mid infrared spectrum for spectrometers operating at all the resolution settings listed in the PREAMBLE, Classification of Data, is a gigantic task, and far beyond the scope of this document.

The verification of resolution is also by no means an easy task. We favor the definition of resolution as the full width at half height of the instrument line shape function, but for many types of spectrometers the width of this function does not remain constant over the entire spectrum. Measurement of the function is not a trivial task, and a spectroscopic determination requires the use of many different compounds for all the resolution settings listed in Table 1 over the entire spectrum. Again the specification of resolution standards is considered to be outside the scope of this document.

Similarly, we have not discussed procedures for sample handling, and good sampling is critical to obtaining accurate quantitative reference spectra. Another parameter necessary for obtaining good quantitative data is cell pathlength. While the pathlength of single-pass cells may be measured fairly accurately, pathlength determination of multi-pass cells is not at all easy, since it is possible that different parts of the beam take different paths. Again, we have not addressed specifications for pathlength determination.

In spite of these limitations, we believe that the specifications above will enable high quality infrared reference spectra of materials in the vapor phase to be measured, collected and used.

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