Pure & Appl. Chem., Vol. 63, No. 12, pp. 1781–1792, 1991.
Printed in Great Britain.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY DIVISION
COMMISSION ON MOLECULAR STRUCTURE AND SPECTROSCOPY*

in conjunction with the

WORKING PARTY ON INFRARED COMPUTERIZED DATA BANKS†

JCAMP-DX, A STANDARD FORMAT FOR EXCHANGE OF INFRARED SPECTRA IN COMPUTER READABLE FORM

(IUPAC Recommendations 1991)

Prepared for publication by
JEANETTE G. GRASSELLI
Ohio University, Athens, Ohio 45701, USA

*Membership of the Commission during the preparation of this report (1983–89) was as follows:

Chairman: J. R. Durig (USA; 1983–89); *Secretary*: H. A. Willis (UK; 1983–87); J. G. Grasselli (USA; 1987–89); *Titular Members*: A. M. Bradshaw (FRG; 1983–89); R. D. Brown (Australia; 1987–89); B. G. Derendjaev (USSR; 1983–89); J. G. Grasselli (USA; 1983–89); E. Hirota (Japan; 1985–89); J. F. J. Todd (UK; 1983–89); *Associate Members*: R. D. Brown (Australia; 1983–87); S. Forsen (Sweden; 1983–87); R. K. Harris (UK; 1983–89); H. Kon (USA; 1983–87); S. Leach (France; 1987–89); G. J. Martin (France; 1985–89); L. N. Masalov (USSR; 1987–89); Yu N. Molin (USSR; 1983–87); W. B. Person (USA; 1983–89); C. J. H. Schutte (RSA; 1983–89); M. Tasumi (Japan; 1983–87); S. Tsuchiya (Japan; 1987–89); *National Representatives*: J. E. Collin (Belgium; 1985–89); R. Colin (Belgium; 1983–85); S. L. Spassov (Bulgaria; 1987–89); G. Herzberg (Canada; 1983–87); Y. Kawano (Brazil; 1983–85); J. Lu (Chinese Chemical Society; 1983–89); G. Varsanyi (Hungary; 1985–89); M. Chowdhury (India; 1986–89); Z. Luz (Israel; 1983–89); S. Ng (Malaysia; 1983–89); B. Jezowska-Trzebiatowska (Poland; 1983–89); T. A. Ford (RSA; 1987–89); C. Pascual (Spain; 1987–89); M. Cebe (Turkey; 1987–89).

†Membership of the Working Party is as follows:

Chairman: J. G. Grasselli (USA); *Members*: B. G. Derendjaev (USSR); M. Ford (UK); P. R. Griffiths (USA); K. Holland-Moritz (Germany); H. Matsuura (Japan); R. S. McDonald (USA).

JCAMP-DX, a standard format for exchange of infrared spectra in computer readable form (Recommendations 1991)

Abstract - The project committee recommends the use of JCAMP-DX to standardize infrared spectral data for ease in transmission between infrared spectrometer data systems and between such systems and other computers. JCAMP-DX is a standard file format that supplies specifications for encoding digitized spectral data, including all the information needed to plot and label a spectrum, as well as additional information about a sample (such as sample preparation and properties), instrumental parameters, and sampling and computational procedures. The digital output (the spectra, interferograms, transformed spectra, and peak tables) from any type of infrared spectrometer can be handled using JCAMP-DX. Data encoded using JCAMP-DX specifications consist of printable ASCII characters and are acceptable to all computers and data systems. The committee recommends that data be carefully documented within JCAMP-DX files. IUPAC-acceptable names and units should be used. Restrictions are applied to some of the JCAMP-DX specifications and additional requirements are given in order to meet IUPAC standards.

PREAMBLE

Introduction

In order for digitally stored infrared data to be readily transmitted from one computer to another (such as between one spectrometer data system and another of a different make) it is necessary to format the data in a uniform and compatible manner.

JCAMP-DX provides such a format (Ref.1), and the project committee recommends its use with some restrictions, which are given later. It is a file format that allows one to standardize spectral data. First priority is given to representing this spectral data without loss of significant detail. JCAMP-DX also allows one to standardize descriptive information (about a sample, instrument, and procedures), which is normally absent from or very abbreviated in *internal* files. *Internal* files refer to those generated by individual spectrometric systems. JCAMP-DX is an *external* format that allows exchange of data between systems which use different *internal* formats.

JCAMP-DX was developed by the Joint Committee on Atomic and Molecular Physical Data (JCAMP) with assistance from a number of infrared spectrometer manufacturers. It is copyrighted by JCAMP, and has been placed in the public domain. Although it was designed for infrared spectra, JCAMP-DX is readily applicable to other types of data, e.g., Raman, NMR, X-ray powder patterns, ultraviolet/visible, ESCA, TGA, chromatograms, etc. Future documents will give specifications for the storage of other types of data. This paper deals specifically with infrared data.

All data transmitted using JCAMP-DX are represented as printable ASCII characters and are compatible with all media (telephone, magnetic and optical disk, magnetic tape, and even the printed page, via optical reader).

JCAMP-DX permits freedom of choice of the encoding interval, thus accommodating rational wavenumber or laser abscissa intervals. The burden of interpolation, if necessary, is placed on the receiving system.

When a JCAMP-DX file is received by an end-user, the receiving system software automatically handles problems due to the *internal* incompatibility of the systems, such as different sequencing of the data, different spacing, and excessive dynamic range. The end-user can make decisions about handling an excessively large file and employ techniques such as truncation and text editing.

Additional advantages and limitations of JCAMP-DX

Additional Advantages. Organizations which employ JCAMP-DX have the freedom to choose infrared spectrometers on the basis of performance rather than data compatibility. They can employ many different makes of spectrometers and still be able to transmit data between them (Ref.1).

A JCAMP-DX spectrum is a text file and hence can be edited and manipulated by a word processor. Record keeping can be facilitated with the use of JCAMP-DX as it provides the ability to combine unlimited amounts of descriptive information with spectral data.

The publication of digital spectra in public databases for use by the scientific community may be facilitated by the use of JCAMP-DX. JCAMP-DX is seen as a format which contributors could use to submit such information.

Limitations. JCAMP-DX is not designed for applications which require the rapid search of very large databases. Such applications require random access and avoidance of arithmetic operations such as ASCII-to-binary conversion. JCAMP-DX files can however be used to transmit or archive data that ultimately are a source for a database application.

IUPAC recommendations

The project committee recommends that in the use of JCAMP-DX, several points be considered (Refs.2,3).

Samples and spectra should be carefully documented in the NOTES (see section below on the NOTES portion of a JCAMP-DX file). Much of this information must be added manually because it is not normally contained in internal spectrometer data files.

IUPAC names of chemicals and units should be used (Refs.4,5).

The committee recommends that data manipulation for cosmetic purposes be kept to a minimum, i.e. smoothing, deconvolution, baseline flattening. However, instrumental background, atmospheric absorption, etc., should be removed when possible by taking the ratio of sample data to a suitable blank. Apodization may be used if appropriate. All such data manipulation should be fully documented under ##DATA PROCESSING= (Section 7.4.6 in (Ref.1)).

Correction for solvent absorption is acceptable if allowance is made for dilution by the solute. In regions of total absorption by the solvent, ordinates should be represented by the JCAMP-DX symbol ('?') for invalid data.

Impurity bands should not be subtracted from reference spectra; they should be carefully documented under ##CONCENTRATIONS=.

The full precision of the data should be retained, but ordinate data should be rounded to the precision warranted by the measurement, both to reduce file size and to show the originator's estimate of precision.

The choice of ordinate units depends mainly on the type of measurement and the intended use of the data. Either transmittance or absorbance can be used for transmission spectra, but absorbance should be used only for high quality data in which no absorption bands are totally absorbing since such regions cannot be represented in absorbance.

The JCAMP-DX ASDF (ASCII Squeezed Difference Forms) compression algorithms, including the "squeezed", "difference", and "duplicate-suppression" forms, as described in Section 5 of (Ref.1) are precise. The combination of these three forms reduces file size significantly, and offers a degree of protection against data transmission errors. However, file transfer should always be protected by a more rigorous error-detection/correction mechanism. Most media (disk, tape, LAN, etc.) provide for error correction automatically. Transfers via media which do not provide such error correction (most modems, optical reader, etc.) should employ an external error-correcting protocol such as Kermit (Ref.6) to preserve the integrity of the data.

The inclusion of certain pieces of information not required by JCAMP is recommended, e.g., IUPAC names. Some of the specifications have been made more restrictive (required vs. optional) in order to comply with IUPAC standards relating to documentation. See "Specifications" at the end of this paper.

Previous specifications for infrared spectra approved by IUPAC

A previous article described specifications for infrared reference spectra of molecules in the vapor phase (Ref.7). This article also described data storage on magnetic tape using FORTRAN, where descriptive information was written as ASCII Variable Block Size records, and spectral data was written as unformatted binary records. Because the internal representation of binary numbers differs among computers of different manufacture, there were complications in processing the latter records in many computer systems. However, most of the descriptive information and the method of presentation suggested in (Ref.7)

are also pertinent for JCAMP-DX files. The use of JCAMP-DX allows one to take this basic information and place it in formatted records using printable ASCII characters which are accepted by all systems and readable by humans. It also provides a more generalized format that allows representation of data other than vapor phase spectra, and of data presented in a variety of ways (such as infrared peak tables, interferograms, and transformed spectra).

STRUCTURE OF JCAMP-DX FILES

A JCAMP-DX file can be either simple or compound. See Section 3 of (Ref.1). A simple file is composed of a single "block" that consists of information to plot and label one spectrum. A compound JCAMP-DX file consists of multiple blocks, each containing a spectrum or fragment of a spectrum, all nested within a *link* block. Each *data* block of a compound file is a complete simple JCAMP-DX file which can be extracted and processed separately.

A compound file, for example, might consist of all data from a Gas Chromatography/ Infrared (GCIR) run in *N*+1 *data* blocks within a *link* block, one *data* block containing the chromatogram and the remaining *N* *data* blocks containing spectra of the *N* fractions. (See Table XI of (Ref.1) for the schematic of a compound file with multiple data blocks nested in a link block.) High resolution vapor spectra which contain a few widely separated absorbing regions can be represented as several blocks, one for each absorbing region. Another example is the combination of sample and reference interferograms as separate blocks within a *link* block in a compound file.

Each block contains individual pieces of information called Labeled-Data-Recoeds (LDRs). All data in the file are free form. Each LDR takes as many lines as necessary and contains a *data-label-flag* (##), a *data-label-name* (for example, TITLE), a *data-label-terminator* (=), and a *data-set* (which is the information to be encoded). The data-set can be text, ASCII string, or numeric. The distinction between text and string is that text is intended to be read by humans, while ASCII string information is structured for possible reading by computer. The column in which data begins is *insignificant*; however, *order* of data elements is important. Each LDR ends with the next data-label-flag (##).

Reserved labels are defined in JCAMP-DX and are global in scope. Users can also generate their own labels as needed. The first character of the *data-label-name* of such *user-defined data-labels* is always $ (which is not allowed in reserved data labels). This is to prevent an accidental collision between a user-defined data-label and any subsequent addition to the list of reserved data-labels. Thus, a user may define the label, ##$OPERATOR'S NAME=, for an LDR containing the operator's name.

An LDR which starts with ##= (i.e., a data-label without a name) is a comment. Such comments can continue for more than one line and are terminated by the next data-label-flag (##). Short comments can be inserted at any point in a line by prefixing them with $$; these comments continue only to the end of the current line and do not terminate an LDR. (See Table III and IV of (Ref.1) for ASCII printing characters and special characters.)

SPECIFICATIONS

CORE portion

A JCAMP-DX file containing data for a spectrum (or an interferogram, peak table, or transformed spectrum) *must* contain a set of LDRs called CORE data. The CORE contains all the information required to plot and label a spectrum. This information can always be generated automatically by software from data in *internal* files. For a detailed description and explanation, see Sections 3.4 and 6 of (Ref.1). Table 1 is an example of CORE data for a spectrum. The LDRs, in the required order for encoding data from a spectrum are listed in the first column. The second column gives an example of the data in JCAMP-DX format, as well as the Section in (Ref.1) where further information can be obtained. The third column gives comments on what is required for an IUPAC-acceptable LDR.

Table 2 is an example of CORE data for a file containing an interferogram. For Fourier domain data (interferograms and transformed spectra), *R* is used for the abscissa and *A* for the ordinate, where *R* is *optical retardation* and *A* is signal *amplitude*. Note that the *X*-limits are also required to define the *X*-region of valid data. As in Table 1, label names, JCAMP-DX examples, and notes on IUPAC-acceptable records are included in Table 2.

For examples of JCAMP-DX files containing a peak table and a transformed spectrum, see Tables VIII and IX, respectively, of (Ref.1).

TABLE 1. Spectrum File. CORE Portion: Examples of Required Labeled-Data-Records (LDRs).

JCAMP-DX	NOTES FOR IUPAC LDR (Refs.2,7)
##TITLE= 1-chloro-2,3-epoxypropane (Epichlorohydrin) vapor	
Should be suitable as a title for a plot of the spectrum. See Section 6.1.1 in (Ref.1).	Name should conform with nomenclature used by IUPAC (Ref.4).
##JCAMP-DX= 4.24	
4.24 is the latest version of JCAMP-DX. See Section 6.1.2 in (Ref.1).	Same as JCAMP-DX.
##DATA TYPE= INFRARED SPECTRUM	
See Section 6.1.3 in (Ref.1).	Same as JCAMP-DX.
**********	
INSERT APPROPRIATE ITEMS FROM NOTES PORTION HERE. SEE TABLE 3.	
**********	
##XUNITS= 1/cm	
See Section 6.2.1 in (Ref.1).	The use of wavenumbers in units of 1/cm is recommended (Ref.5).
##YUNITS= ABSORBANCE	
See Section 6.2.2 in (Ref.1).	It is recommended that spectra be encoded using transmittance, reflectance, absorbance, Kubelka-Munk, or other IUPAC-recommended ordinate scales.
##XFACTOR=[&] 1.0	
##XFACTOR= is a factor by which X-components of ##XYDATA= must be multiplied to obtain actual values. See Section 6.2.5 in (Ref.1).	Same as JCAMP-DX.
##YFACTOR= 0.001	
##YFACTOR= should be chosen to convert Y-values to integers to reduce space required by a block of spectral data without degrading the precision of the data. Section 6.2.5 in (Ref.1).	For the absorbance range 0.0/3.000, ##YFACTOR= could be .001 to convert Y-range to 0 to 3000 if this represents the true precision of the data.
##FIRSTX=[&&] 450	
First actual abscissa value of ##XYDATA=. See Section 6.2.3 in (Ref.1).	Same as JCAMP-DX.
##LASTX=[&&] 4000	
Last actual abscissa value of ##XYDATA=. See Section 6.2.3 in (Ref.1).	Same as JCAMP-DX.

Table 1 (contd.)

##NPOINTS= 1842		
	Number of components of ##XYDATA=, ##XYPOINTS=, etc. See Section 6.2.6 in (Ref.1).	IUPAC recommends that at least two data points per resolution element be used.
##FIRSTY= 0.058		
	Actual Y-value corresponding to ##FIRSTX=. See Section 6.2.7 in (Ref.1).	Same as JCAMP-DX.
##MAXX= 4000 ##MINX= 450		
	##MAXX and/or ##MINX= are required if ##FIRSTX= and ##LASTX= do not span the full range of X. See Section 6.2.4 of (Ref.1).	Same as JCAMP-DX.
##MAXY= 0.3768 ##MINY= -0.0021		
	The largest and smallest actual Y-values. These are optional except in the case where Y-range exceeds recommended ordinate scaling. See Section 6.2.4 in (Ref.1).	Same as JCAMP-DX.
##XYDATA= (X++(Y..Y)) 450 58 44 34 39 26 .... etc. 3998 16 15 14		
	Contains the spectrum as a table of ordinates at equal X-intervals (X++(Y..Y)). This record will extend over many lines. See Section 6.4.1 in (Ref.1).	Same as JCAMP-DX.
or		
##XYPOINTS= (XY..XY) 450,58 451,44 453,39 .... etc.		
	Contains a table of XY pairs for spectral data not spaced at constant abscissa intervals. See Section 6.4.2 in (Ref.1).	Same as JCAMP-DX.
##END=		
	Last LDR in every JCAMP-DX file. See Section 6.1.5 in (Ref.1).	Same as JCAMP-DX.

[&]Rationally spaced X-values are usually left unscaled (##FACTOR= of 1.0). Laser-spaced X-values normally require several decimal places. Optionally, they can be scaled to integral X-values via a suitable ##FACTOR= to reduce file size. In this case, ##XFACTOR= must be sufficiently precise for accurate reconstruction of X-values.

[&&]JCAMP-DX allows spectra to be tabulated in either increasing or decreasing abscissa sequence. This has no effect on the previous IUPAC recommendation that infrared spectra be *plotted* with high wavenumber to the left except that software for decoding JCAMP-DX must be able to accept *tabulated* data in either order.

TABLE 2. Interferogram File. CORE Portion: Examples of Required Labeled-Data-Records (LDRs).

JCAMP-DX	NOTES FOR IUPAC LDR (Refs.2,7)
##TITLE= Sample interferogram for 1-chloro-2,3-epoxypropane (Epichlorohydrin) vapor	
See Section 6.1.1 in (Ref.1).	Name should conform with nomenclature used by IUPAC (Ref.4).
##JCAMP-DX= 4.24	
See Section 6.1.2 in (Ref.1).	Same as JCAMP-DX.
##DATA TYPE= INFRARED INTERFEROGRAM	
See Section 6.1.3 in (Ref.1).	Same as JCAMP-DX.
**********	
INSERT APPROPRIATE ITEMS FROM NOTES PORTION HERE. SEE TABLE 3.	
**********	
##RUNITS= MICROMETERS	
See Section 8.1 in (Ref.1).	Same as JCAMP-DX.
##AUNITS= ARBITRARY UNITS	
See Section 8.2 in (Ref.1).	Same as JCAMP-DX.
##FIRSTR= 0	
##LASTR= 5183.2749	
First and last actual optical retardation values in ##RUNITS=. See Section 8.3 in (Ref.1).	Same as JCAMP-DX.
##DELTAR= 1.265757	
Optical retardation per data point expressed in ##RUNITS=. See Section 8.4 in (Ref.1).	Same as JCAMP-DX.
##NPOINTS= 4096	
See Section 6.2.6 in (Ref.1).	Same as JCAMP-DX.
##ALIAS= 1/1	
A fraction whose denominator is the number of possible aliases for a given sample, and whose numerator is the number of the alias represented by the data. See Section 8.8 in (Ref.1).	Same as JCAMP-DX.
##ZPD= 250	
The position, approximate or precise, of the zero path difference. See Section 8.9 of (Ref.1).	Same as JCAMP-DX.

Table 2 (contd.)

##RFACTOR= 1.265757		
	##RFACTOR= and ##AFACTOR= are factors by which spectral data in ##RADATA= are multiplied to obtain actual values. Normally, ##RFACTOR= equals ##DELTAR=. See Section 8.6 in (Ref.1).	Same as JCAMP-DX.
##AFACTOR= 1.0		
	This should reflect amplifier gain etc., to allow transmittance to be calculated as the ratio of sample to reference intensity. See Section 8.6 in (Ref.1).	Same as JCAMP-DX.
##FIRSTA= -268		
	Actual A-value corresponding to ##FIRSTR=, i.e., the product of ##AFACTOR and the first A-value in ##RADATA=. See Section 8.7 in (Ref.1).	Same as JCAMP-DX.
##MAXA= 29552 ##MINA= -27430		
	Maximum and minimum amplitude of interferogram ordinate data in ##RUNITS=; required because of the large interferogram amplitude near zero path difference (ZPD). See Section 8.5 in (Ref.1).	Same as JCAMP-DX.
##XUNITS=[%] 1/cm		
	See Section 6.2.1 in (Ref.1).	Same as JCAMP-DX.
##FIRSTX=[%] 449.413		
	See Section 6.2.3 in (Ref.1).	Same as JCAMP-DX.
##LASTX=[%] 4000.355		
	See Section 6.2.3 in (Ref.1).	Same as JCAMP-DX.
##RADATA= (R++(A..A)) 0 -268 38 26 -291 -323 .... etc. 4090 4 -270 -273 -266 -268 -278		
	Contains interferogram as a table of ordinates (*A*) vs. retardation (*R*): (*R*++(*A*..*A*)). Each line of this record starts with an R-value, and is followed by a series of *A* values at equal *R* spacing. See Section 8.10 in (Ref.1).	Same as JCAMP-DX.
##END=		
	See Section 6.1.5 in (Ref.1).	Same as JCAMP-DX.

[%]FIRSTX and LASTX are required for interferograms to give the X-limits of valid data, allowing for source/detector range and window/filter transmission. XUNITS is required to give the units of FIRSTX and LASTX.

NOTES portion

The NOTES portion is the variable, descriptive part of a JCAMP-DX file which complements the CORE portion. The LDRs in NOTES can be added to the CORE portion of all types of files between the ##DATA TYPE= and the spectral data so that they can be viewed without listing all of the latter. See Table 3 for description of LDRs in the NOTES portion. Information for LDRs in the NOTES portion is not needed for plotting and labeling a spectrum, and may not be present in *internal* files. It is the responsibility of the sender to add any missing information which describes the sample, equipment, operating parameters, etc.

TABLE 3. NOTES Portion: Examples of Optional Labeled-Data-Records (LDRs).

JCAMP-DX		NOTES FOR IUPAC LDR (Refs.2,7)
Spectral Parameters		
##RESOLUTION= 4.0		
	Nominal resolution in units specified by ##XUNITS=, as a single number for spectra at constant resolution throughout (FTIR spectra), or as pairs of the form: $R_1,X_1 \ldots R_i,X_i$, where R_i stands for resolution at abscissa X_i. See Section 6.3.1 in (Ref.1).	Required by IUPAC for all types of spectra. It is recommended that nominal resolution be given at 3 wavenumbers (750, 1500, and 3000 cm^{-1}).
##DELTAX= 1.0		
	Nominal spacing between points, mainly for inspection by user. Actual X-values are *calculated* as (LASTX-FIRSTX)/(NPOINTS-1). See Section 6.3.2 in (Ref.1).	Optional.
Miscellaneous		
##CLASS= IUPAC B		
	See Section 7.1.1 in (Ref.1).	The IUPAC Class of digital representation, A, B, or C (Ref.3) is required for spectra of pure compounds.
##ORIGIN= XYZ Research Laboratories		
	Name of organization, name of individual contributor, etc., who generated the data, as appropriate. See Section 7.1.2 in (Ref.1).	Laboratory name is required.
##$OPERATOR'S NAME= Chris Doe		
	User defined JCAMP-DX LDR. See Section 4.4.2 in (Ref.1).	Operator's name is required.
##OWNER= EPA/Public Domain		
	If data is copyrighted, this line should read: Copyright (C) <year> BY <name>. If the data is public, this field should contain the words: "Public Domain", as shown. See Section 7.1.3 in (Ref.1).	Required.
##DATE= 77/08/11		
	Date when spectrum was measured, in the form: YY/MM/DD. See Section 7.1.4 in (Ref.1).	Required.
##TIME= 18:36:00		
	Time when spectrum was measured, in the form: HH:MM:SS. See Section 7.1.5 in (Ref.1).	Optional.

Table 3 (contd.)

##SOURCE REFERENCE= No. 2, EPA Vapor Library	
Adequate information to locate the original spectrum, i.e., own-serial-number, name of file containing spectrum, or library name and serial number of spectrum. See Section 7.1.6 in (Ref.1).	Required.
##CROSS REFERENCE=	
Refers to additional spectra of the same sample; serves to link an interferogram with a spectrum, etc. See Section 7.1.7 in (Ref.1).	Required, if appropriate.
Equipment	
##SPECTROMETER/DATA SYSTEM= ABC 000	
Manufacturer's name, model of the spectrometer, software system, and release number, as appropriate, in the form used by the manufacturer. See Section 7.3.1 in (Ref.1).	Manufacturer and model number of spectrometer are required.
##INSTRUMENT PARAMETERS=	
List of instrumental settings that are *essential* for the application. See Section 7.3.1 in (Ref.1).	Required.
Sample Information	
##SAMPLE DESCRIPTION=	
If the sample is not a pure compound, include here a description, i.e., composition, origin, appearance, results of interpretation, etc. For pure compounds, this field may be replaced or supplemented by LDRs listed below. See Section 7.2.1 in (Ref.1).	Required for samples that are not pure compounds. It is recommended that a description of pure compounds be included here also, specifically, the source and tests done to determine purity, etc.
##IUPAC NAME= 1-chloro-2,3-epoxypropane	
See (Ref.4). Replaces ##CAS NAME=. See Section 7.2.2 in (Ref.1).	Required for pure compound.
##NAMES= Epichlorohydrin	
Common, trade, or other names. Multiple names are placed on separate lines. See Section 7.2.3 in (Ref.1).	Required, if applicable.
##MOLFORM= C3 H5 Cl O	
See Section 7.2.4 in (Ref.1).	Required for pure compound.
##CAS REGISTRY NO= 13403-37-7	
See Section 7.2.5 in (Ref.1).	Connectivity matrix (that describes structural features) and/or CAS Registry Number is required for pure compound.
##BEILSTEIN REGISTRY NO= 1420785	
Searchable as BRN for the substance record in the Beilstein file.	Required for a pure compound.

Table 3 (contd.)

##WISWESSER= T3OTJ B1G See Section 7.2.6 in (Ref.1).	Optional.
##BEILSTEIN LAWSON NO= 16782 Structural formula clustering code. Searchable as LN for specific fragments of molecules. See Section 7.2.7. in (Ref.1).	Optional.
##MP=@ -48C $$ CRC Handbook value. See Section 7.2.8 in (Ref.1).	Required for a pure compound.
##BP=@ 116.5C^760mm $$ CRC Handbook value See Section 7.2.9 in (Ref.1).	Required for a pure compound.
##REFRACTIVE INDEX=@ ND=1.4361^20 $$CRC Handbook value Index at 20°C for Na D line. See Section 7.2.10 in (Ref.1).	Desirable.
##DENSITY=@ 1.1801^20/4 $$ CRC Handbook value Density at 20°C in kg/m^3. See Section 7.2.11 in (Ref.1).	Desirable.
##MW= 92.53 Molecular weight. See Section 7.2.12 in (Ref.1).	Desirable.
##CONCENTRATIONS= List of known components and impurities and their concentrations in the form $(N_1,C_1,U_1),\ldots,(N_i,C_i,U_i)$, where N stands for name, C for concentration, and U for units of concentration. See Section 7.2.13 in (Ref.1).	Desirable.
Sampling Information	
##SAMPLING PROCEDURE= MODE: transmission ACCESSORIES: GC capillary flow cell	
$$ Other sampling information, as appropriate. First entry is MODE of observation, followed by appropriate additional information. The following LDRs are used in place of, or to supplement this LDR. See Section 7.4.1 in (Ref.1).	Required. MODE should be included here. Other parameters, such as path length, pressure, etc., are included below.
##STATE= gas Specify here if sample is solid, liquid, gas, KBr pellet, etc. See Section 7.4.2 in (Ref.1).	Required.
##PATH LENGTH= 7.6 cm See Section 7.4.3 in (Ref.1).	Required, if appropriate (e.g., gas phase, liquid cells).

Table 3 (contd.)

##PRESSURE= Unknown		
	Sample pressure in appropriate units. See Section 7.4.4 in (Ref.1).	Partial pressure (kPa) of all gaseous samples is required including samples at atmospheric pressure. Pressure in appropriate units is also required for condensed phases if significantly different from atmospheric.
##$PRESSURE BROADENING GAS= Helium, 1 atmosphere		
	IUPAC-defined JCAMP-DX LDR. See Section 4.4.2 in (Ref.1).	Partial pressure (kPa) of broadening gas, if applicable, is required.
##TEMPERATURE= 200°C		
	See Section 7.4.5 in (Ref.1).	Required for all samples.
##DATA PROCESSING=		
APODIZATION: NONE $$ or apodizing function ZERO FILL: 1X BACKGROUND: EMPTY CELL $$ or alternative SMOOTHING: NONE $$ or smoothing function $$ Other details, as appropriate		
	See Section 7.4.6 in (Ref.1).	Required. It is recommended that data processing be kept to a minimum.

[@]Preferably *actual* value for sample. If value is from a handbook, this should be noted as a $$ comment as shown in examples.

CONCLUSIONS

IUPAC recommends the use of JCAMP-DX for encoding digitized spectral data in a standard format for transmission between data systems and computers. However, in some cases, IUPAC has defined more restrictive subsets of the JCAMP-DX LDRs and recommended the inclusion of other records not required by JCAMP-DX. The use of JCAMP-DX should facilitate the processing and interpretation of infrared data, as more data is exchanged between spectroscopists and users of personal computers.

Acknowledgements

Special thanks to Dr. D. Cameron for detailed review and recommendations pertaining to this document, to Dr. C. Anderson for helpful discussions and contributions, and to M. Schiele for editorial help.

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