

JCAMP-DX for Mass Spectrometry

PETER LAMPEN,* HEINRICH HILLIG, ANTONY N. DAVIES,
and MICHAEL LINSCHIED

Institut für Spektrochemie und Angewandte Spektroskopie, ISAS, Postfach 10 13 52, 44013 Dortmund, Germany

JCAMP-DX has, for several years, been the standard form for the exchange of infrared spectral data. More recently JCAMP-DX protocols have been published for chemical structure data and for nuclear magnetic resonance spectroscopy. This publication presents a new JCAMP-DX data exchange protocol for mass spectrometry, covering the transport of single spectra, spectral series, and raw data files. The protocol can be implemented on any computer system and storage media. It is completely manufacturer independent. As with previous publications in this series, the aim is to provide reliable data transfer without loss of information regardless of the hardware or software involved. A comparison to the work on a binary protocol currently being carried out by the Analytical Instrument Association is also presented.

Index Headings: JCAMP-DX for MS; Mass spectra data exchange; Data exchange; Data processing.

1. INTRODUCTION

The JCAMP-DX format has been used effectively for data exchange in the field of infrared spectroscopy^{1,2} and more recently for nuclear magnetic resonance spectroscopy.³ A similar powerful and flexible standard format for mass spectrometry (MS) has been sorely missed. As program packages from independent software houses have grown in popularity, the need to exchange spectroscopic data between spectrometers and personal computers or workstations has become increasingly important. Data exchange can be simplified if a generally accepted exchange standard is available.

Additionally, there are many collections of mass spectrometric data within the chemical industry, measured for the most part on old spectrometers, no longer supported by their manufacturers. There is enormous interest in the introduction of an appropriate, easy-to-implement format for the conversion and archiving of such data.

A data standard ought to be in the "public domain" and be capable of extension to meet the individual requirements of implementers without breaching the core information content.

A committee of representatives of mass spectrometer manufacturers under the auspices of the American Society for Mass Spectrometry (ASMS) started work on a definition based on the JCAMP-DX infrared protocol, Version 4.24.^{4,5} However, a decision was made at the

ASMS conference in May 1991 to abandon this work, and instead to base the further development of a data exchange format on the public domain netCDF (network Common Data Form) package supported by the Unidata Program Center.⁶ The netCDF program library has been extended by a second subroutine collection called *andi/MS* (analytical data interchange for mass spectrometry).⁷ Implementations of this protocol are being incorporated into current mass spectrometry data system software by vendors and other third parties.

Although the *andi/MS* protocol has recently been accepted by the governing board of the Analytical Instrument Association (AIA), we believe that a definition of a JCAMP-DX format for mass spectrometry is not only relevant but urgent. The reasons for this belief are that JCAMP-DX is, as opposed to *andi/MS*, extremely simple to implement. The necessary software modules can be written in any computer language, even in BASIC or ASSEMBLER. This possibility is very important for accessing spectral data on systems no longer supported by the vendors and for making the existing large data collections available in a unique format. JCAMP-DX uses exclusively ASCII characters. ASCII formats are advantageous because of their hardware and operating system independence. The use of exclusively ASCII characters for the protocol is safe for adoption in long-term archiving, an essential point for laboratories facing accreditation.

The definition of JCAMP-DX for mass spectrometry completes the definition of uniform data exchange protocols for the most wide-spread molecular spectroscopy methods.⁸ STN International has adopted JCAMP-DX as download format for mass spectral data in addition to IR and NMR spectra, as well as for chemical structures.

Because of the open structure of JCAMP-DX for MS, the convertibility between *andi/MS* and JCAMP-DX can be achieved without loss of information. This capability ensures that the coexistence of both transport formats will not cause any problems.

The JCAMP-DX for MS protocol was developed in collaboration with the chemical industry for organic mass spectrometry. The authors have defined *labeled-data-records* for mass spectrometry on the basis of the draft "Generic JCAMP-DX, Version 5.0".⁹ The difficult task of handling multidimensional mass spectra (MS/MS measurements) was deliberately left out since the develop-

Received 16 March 1994; accepted 11 August 1994.

* Author to whom correspondence should be sent.

ments of JCAMP-DX Version 5.0 in this area are still not complete. The definitions published here cover single spectra, spectral series (e.g., GC/MS measurements), and continuous mass spectra (*raw data*), i.e., data with constant abscissa increment and without peak detection.

2. SCOPE

This document was presented to the Joint Committee on Atomic and Molecular Physical Data (JCAMP) working group on Data Exchange (DX) and the JCAMP executive on 2 March 1994 in Chicago, where it was accepted and given free for publication. A draft version had previously been presented for comment at the 8th workshop, "Computer in Chemistry", in Seeheim/Jugenheim, Germany (1993). The protocol is meant for public use. The specifications are placed in the public domain, and the right to copy for scientific purposes is hereby granted.

3. FILE STRUCTURE AND DEFINITIONS

This publication is oriented as far as possible towards the JCAMP-DX Version 4.24 protocol for infrared spectra.¹ Since spectral series are extremely inefficiently handled in the infrared protocol, the draft JCAMP-DX Version 5.0⁹ was resorted to for data of this type. This new version allows data storage with more than one independent variable in the *NTUPLE* format. An example is a GC/MS measurement, where the intensity values are dependent on the mass-to-charge ratio m/z and on the retention time t .

(3.1) CORE AND NOTES. A JCAMP-DX file consists of *core* and *notes* portions. The core portion is the irreducible minimum JCAMP-DX file. It contains all information required to identify and represent the spectral data itself. The notes portion complements the core portion. Notes describe the sample in greater detail than does the `##TITLE=` (see 5.1), as well as describing equipment, sampling parameters, data processing, and any additional details which are appropriate for a particular spectrum.

(3.2) LABELED-DATA-RECORDS. Within a JCAMP-DX file, data are stored in *labeled-data-records* (LDRs; see Ref. 1, section 4.2). Each record begins with the *data label flag* (`##`). There then follows a *label name*, which ends with the *data label terminator* (`=`). Following the equals sign is the *data set* part of the record. Each record has the format "`##labelname= data set`". Data-type-specific records are written in the JCAMP-DX Version 5.0 format "`##.labelname data= set`" with an extra period (`.`) between the data label flag and the label name. Each record can consist of many lines, each up to 80 characters long and ending in CR LF (ASCII 0x13, 0x10).

(3.3) USER-DEFINED LABELS. The user of JCAMP-DX for MS is free to define additional *user-defined labels* to handle spectral information which is not covered by the labels listed below. These labels take the format "`##$labelname=`".

(3.4) COMMENTS. Comments may be inserted as comment records flagged with the data label "`##=#`", which allows the comment to carry over several lines until the next data record. A second possibility is to insert comments inside other records in the format "`$$ comment`" as advised inside the `##JCAMP-DX=` record to identify

software (see 5.1.1). These comments finish at the end of the line in which they start.

4. DATA REPRESENTATION

The following *data forms* are used, as in infrared spectroscopy, as data sets. In the record definitions below they will always be written in parentheses.

- Text** A data set containing written information not specially intended to be read by computer systems.
- String** A pre-defined text (e.g., "MASS SPECTRUM"). Strings have to be implemented exactly as specified in the definition since they are intended to be read by humans and computers alike.
- AFFN** *ASCII free format numeric*: An integer or a real number in fixed point or scientific notation.
- ASDF** *ASCII squeezed difference form*: Tabular data using the JCAMP-DX data compression scheme (see section 4.2).

(4.1) TABULAR DATA. The actual spectral data, peak tables, or raw data, are stored in *data tables*. The format of the data table used is described symbolically in the so-called *variable-list* (see Ref. 1, section 5.1.1), which is placed following the data label terminator. The spectral data begin on the next line. For mass spectra two table formats are relevant, as described below.

Peak lists are stored in the format: " $x_1, y_1; x_2, y_2; \dots x_n, y_n$ ". The relevant variable-list is: "(XY..XY)". A comma is used as the separator between X- and Y-values, and a space, semi-colon, or end of line (CR LF) is used between XY data pairs. One is not allowed to separate an XY data pair with an end of line. To ease file readability, the authors recommend that each data pair be presented on a separate line. Since CR LF does not take up more memory than a semicolon and space, the file size would not be increased by adopting this strategy.

Data where X-values vary with a constant increment (e.g., raw data) are stored in lines beginning with a single X-value and continuing with Y-values up to the end of the line: " $x_1, y_1, y_2, \dots y_n$ ". The following X-values can be calculated from the initial X-value and the increment. The next line again begins with an X-value (*X-sequence-check*; see Ref. 1, section 5.8.1). The type of data table is defined by the variable-list "(X+(Y..Y))". In addition the JCAMP-DX Version 4.24 data compression scheme (ASDF) may be used.

(4.2) DATA COMPRESSION. The data compression scheme uses a combination of the following forms (see Ref. 1, section 5.):

- PAC** Packed form: The values are separated by a +, a -, or a blank.

TABLE I. Pseudo-digits.

ASCII	0	1	2	3	4	5	6	7	8	9
Positive SQZ	@	A	B	C	D	E	F	G	H	I
Negative SQZ		a	b	c	d	e	f	g	h	i
Positive DIF	%	J	K	L	M	N	O	P	Q	R
Negative DIF		j	k	l	m	n	o	p	q	r
Positive DUP		S	T	U	V	W	X	Y	Z	s

TABLE II. Fixed header labeled-data-records.

Label (data form)	Content
##TITLE= (text)	e.g., (Sample name)
##JCAMP-DX= (string)	5.00 \$\$ (Name and version number of the JCAMP-DX program)
##DATA TYPE= (string)	e.g., MASS SPECTRUM
##DATA CLASS= (string)	e.g., PEAK TABLE
##ORIGIN= (text)	e.g., (Chemist-Name)
##OWNER= (text)	e.g., COPYRIGHT (C) (Year) by (Name)

SQZ Squeezed form: The separator, the initial digit, and the sign of the number are combined into a *pseudo-digit* (see Table I).

DIF Difference form: The first Y-value in each line is in SQZ form; the following Y-values are stored as differences. Pseudo-digits are used. The last Y-value in any line is used, together with the appropriate X-value, as the first data pair in the following line (*Y-value-check*; see Ref. 1, section 5.8.2).

DUP Duplicate suppression: When several Y-values or differences in succession are identical, all except the first occurrence are replaced by a duplicate-count whose initial digit comes from Table I, line 6. Duplicate-count is the number of identical table values including the first one. This method can be combined with the SQZ form (SQZDUP) or the DIF form (DIFDUP).

5. THE CORE

The following section describes the required data labels for the JCAMP-DX file. The file core consists of three parts. The first part is called the *fixed header information*. It consists, with one exception (##DATA CLASS=; see 5.1.3) of well-known labeled-data-records from the JCAMP-DX Version 4.24. The second part is the *variable header information*, and the final part is the *spectral data*.

(5.1) **FIXED HEADER INFORMATION**. These LDRs are necessary and must be used exactly in the order given in Table II.

(5.1.1) The version number in LDR ##JCAMP-DX= is 5.00; it is now very strongly recommended that this information should be followed with a comment (\$\$) on the same line giving the name and version number of the software responsible for producing the JCAMP-DX file.

(5.1.2) For ##DATA TYPE=, the strings "MASS SPECTRUM" for mass spectra and spectral series and "CONTINUOUS MASS SPECTRUM" for raw data are defined.

(5.1.3) The new LDR is the JCAMP-DX Version 5.0 label ##DATA CLASS=, with the help of which single spectra and spectral series will be differentiated. For ##DATA CLASS=, the following strings are defined: "PEAK TABLE" for single spectra, "XYDATA" for raw data, and "NTUPLES" for spectral series given in the new NTUPLE format.

(5.1.4) The two labels ##ORIGIN= and ##OWNER= should be included. Software developers should also ensure that a JCAMP-DX file cannot be created with these fields left blank, nor containing the name of the instrument vendor as fixed value!

(5.2) **VARIABLE HEADER INFORMATION**. The use of ##IONIZATION MODE= is required, and ##SPECTROMETER TYPE= and ##INLET= are strongly recommended. It is recommended that explanatory information be included which appears after the abbreviations in this section as a \$\$ comment in the actual JCAMP-DX files (see example 1).

(5.2.1) ##SPECTROMETER TYPE= (string). The following strings have been defined for the different types of mass spectrometers:

Example 1. Single spectrum.

##TITLE=	2-Chlorophenol
##JCAMP-DX=	5.00 \$\$ ISAS JCAMP-DX program (V.1.0)
##DATA TYPE=	MASS SPECTRUM
##DATA CLASS=	PEAK TABLE
##ORIGIN=	H. Mayer, ISAS Dortmund, Germany
##OWNER=	COPYRIGHT (C) 1994 by ISAS Dortmund, Germany
##SPECTROMETER/DATA SYSTEM=	Finnigan MAT Magnum
##INSTRUMENTAL PARAMETERS=	LOW RESOLUTION
##SPECTROMETER TYPE=	TRAP \$\$ ion trap spectrometer
##INLET=	GC \$\$ gas chromatograph as inlet
##IONIZATION MODE=	EI+ \$\$ electron impact ionization with positive polarity
##.BASE PEAK=	128
##.BASE PEAK INTENSITY=	687729 COUNTS
##.RIC=	3063043
##XUNITS=	M/Z
##YUNITS=	RELATIVE ABUNDANCE
##NPOINTS=	26
##PEAK TABLE=	(XY..XY)
50, 5.84	
51, 9.55	
...	
130, 32.45	
131, 2.13	
##END=	

TABLE III. Labeled-data-records for single spectra.

Label (data form)	Content
##XUNITS= (string)	M/Z
##YUNITS= (string)	RELATIVE ABUNDANCE
##NPOINTS= (AFFN)	(number of data points in the ##PEAK TABLE=)
##PEAK TABLE= (AFFN or ASDF)	(XY..XY)
##END=	

- B for a magnetic sector field spectrometer
- EB for a double-focusing spectrometer with EB geometry
- BE for a double-focusing spectrometer with BE geometry
- Q for a quadrupole spectrometer
- TRAP for an ion-trap spectrometer
- TOF for a time-of-flight spectrometer.

(5.2.2) ##.INLET= (string). In this record the inlet type should be described with the following strings:

- DIRECT for a direct probe
- BATCH for a batch inlet
- GC for a gas chromatograph as inlet system
- LC for a liquid chromatograph as inlet system
- CZE for a capillary-zone electrophoresis system as inlet
- PB for a particle-beam inlet
- MOB for a moving-belt inlet.

(5.2.3) ##.IONIZATION MODE= (string). The type of ionization is given in the following strings. The polarity is registered with the appropriate sign tagged onto the relevant string.

- EI+ or EI- for electron impact ionization
- CI+ or CI- for chemical ionization
- FAB+ or FAB- for fast atom bombardment
- TSP+ or TSP- for thermospray ionization
- ESI+ or ESI- for electrospray ionization
- APICI+ or APICI- for atmospheric pressure ionization with chemical ionization
- LD+ or LD- for laser desorption.

Extra information may be added following the string by use of the \$\$ comment (e.g., "CI+ \$\$" (Reaction gas) or "FAB- \$\$" (Matrix)/(primary particle)).

(5.2.4) ##BLOCKS= (AFFN) and ##BLOCK_ID= (AFFN). These records are to be used in *compound JCAMP-DX files* as defined in Version 4.24 and as extended in the

JCAMP-CS protocol to provide inter-block referencing (see Ref. 10, section 5.13). A unique positive integer must be given to each block within a compound file. This number must not necessarily be sequential. For ease of use it is recommended that separate files be used for each data block or the NTUPLE format for spectral series instead of compound files.

(5.3) SPECTRAL DATA. The records ##DATA TYPE= and ##DATA CLASS= provide information about the type of data stored in the JCAMP-DX file.

(5.3.1) SINGLE SPECTRA. Single spectra can be recognized by the records ##DATA TYPE= MASS SPECTRUM and ##DATA CLASS= PEAK TABLE. The data will be stored in the LDRs given in Table III (also see example 1). The Y-values in the ##PEAK TABLE= a normalized to the intensity of the base peak of the spectrum (Y-value of the base peak is set to 100.0).

(5.3.2) RAW DATA. For raw data the records ##DATA TYPE= CONTINUOUS MASS SPECTRUM and ##DATA CLASS= XYDATA are to be used. The records required for raw data files are given in Table I (also see example 2).

(5.3.3) SPECTRAL SERIES. Spectral series can be recognized by the use of the records ##DATA TYPE= MASS SPECTRUM and ##DATA CLASS= NTUPLES. These series are stored in the new JCAMP-DX Version 5.0 defined NTUPLE format. The LDRs in Table V are used to produce the NTUPLE structure (also see example 3).

The LDRs forming the *data page* must be repeated for each of the spectra in the series. The value for the retention time in the ##PAGE= record will be used as the *page attribute*. The actual value for the second independent variable (and possibly other variables) should be given here. The method of displaying the data will appear in the record ##DATA TABLE= following the variable-list "(XY..XY)". Apart from "PEAKS", the strings "XY-DATA", "PROFILE", and "CONTOUR" are allowed. The next line must contain the first XY data pair. Since the number of peaks in each mass spectrum of the spectral

TABLE IV. Labeled-data-records for raw data.

Label (data form)	Content
##XUNITS= (string)	SECONDS, CHANNEL NUMBER or ARBITRARY UNITS
##YUNITS= (string)	COUNTS or ARBITRARY UNITS
##XFACTOR= (AFFN)	(Factor by which the X-values in ##XYDATA= must be multiplied to obtain the original values)
##YFACTOR= (AFFN)	(Factor by which the Y-values in ##XYDATA= must be multiplied to obtain the original values)
##FIRSTX= (AFFN)	(Unscaled first X-value in ##XYDATA=)
##LASTX= (AFFN)	(Unscaled last X-value in ##XYDATA=)
##NPOINTS= (AFFN)	(Number of data points in ##XYDATA=)
##FIRSTY= (AFFN)	(Unscaled first Y-value in ##XYDATA=)
##XYDATA= (AFFN or ASDF)	(X++(Y..Y))
##END=	

TABLE III. Labeled-data-records for single spectra.

Label (data form)	Content
##XUNITS= (string)	M/Z
##YUNITS= (string)	RELATIVE ABUNDANCE
##NPOINTS= (AFFN)	(number of data points in the ##PEAK TABLE=)
##PEAK TABLE= (AFFN or ASDF)	(XY..XY)
##END=	

- B for a magnetic sector field spectrometer
- EB for a double-focusing spectrometer with EB geometry
- BE for a double-focusing spectrometer with BE geometry
- Q for a quadrupole spectrometer
- TRAP for an ion-trap spectrometer
- TOF for a time-of-flight spectrometer.

(5.2.2) ##.INLET= (string). In this record the inlet type should be described with the following strings:

- DIRECT for a direct probe
- BATCH for a batch inlet
- GC for a gas chromatograph as inlet system
- LC for a liquid chromatograph as inlet system
- CZE for a capillary-zone electrophoresis system as inlet
- PB for a particle-beam inlet
- MOB for a moving-belt inlet.

(5.2.3) ##.IONIZATION MODE= (string). The type of ionization is given in the following strings. The polarity is registered with the appropriate sign tagged onto the relevant string.

- EI+ or EI- for electron impact ionization
- CI+ or CI- for chemical ionization
- FAB+ or FAB- for fast atom bombardment
- TSP+ or TSP- for thermospray ionization
- ESI+ or ESI- for electrospray ionization
- APICI+ or APICI- for atmospheric pressure ionization with chemical ionization
- LD+ or LD- for laser desorption.

Extra information may be added following the string by use of the \$\$ comment (e.g., "CI+ \$\$" (Reaction gas) or "FAB- \$\$" (Matrix)/(primary particle)).

(5.2.4) ##BLOCKS= (AFFN) and ##BLOCK_ID= (AFFN). These records are to be used in *compound JCAMP-DX files* as defined in Version 4.24 and as extended in the

JCAMP-CS protocol to provide inter-block referencing (see Ref. 10, section 5.13). A unique positive integer must be given to each block within a compound file. This number must not necessarily be sequential. For ease of use, it is recommended that separate files be used for each data block or the NTUPLE format for spectral series instead of compound files.

(5.3) SPECTRAL DATA. The records ##DATA TYPE= and ##DATA CLASS= provide information about the type of data stored in the JCAMP-DX file.

(5.3.1) SINGLE SPECTRA. Single spectra can be recognized by the records ##DATA TYPE= MASS SPECTRUM and ##DATA CLASS= PEAK TABLE. The data will be stored in the LDRs given in Table III (also see example 1). The Y-values in the ##PEAK TABLE= are normalized to the intensity of the base peak of the spectrum (Y-value of the base peak is set to 100.0).

(5.3.2) RAW DATA. For raw data the records ##DATA TYPE= CONTINUOUS MASS SPECTRUM and ##DATA CLASS= XYDATA are to be used. The records required for raw data files are given in Table IV (also see example 2).

(5.3.3) SPECTRAL SERIES. Spectral series can be recognized by the use of the records ##DATA TYPE= MASS SPECTRUM and ##DATA CLASS= NTUPLES. These series are stored in the new JCAMP-DX Version 5.0 defined NTUPLE format. The LDRs in Table V are used to produce the NTUPLE structure (also see example 3).

The LDRs forming the *data page* must be repeated for each of the spectra in the series. The value for the retention time in the ##PAGE= record will be used as the *page attribute*. The actual value for the second independent variable (and possibly other variables) should be given here. The method of displaying the data will appear in the record ##DATA TABLE= following the variable-list "(XY..XY)". Apart from "PEAKS", the strings "XY-DATA", "PROFILE", and "CONTOUR" are allowed. The next line must contain the first XY data pair. Since the number of peaks in each mass spectrum of the spectral

TABLE IV. Labeled-data-records for raw data.

Label (data form)	Content
##XUNITS= (string)	SECONDS, CHANNEL NUMBER or ARBITRARY UNITS
##YUNITS= (string)	COUNTS or ARBITRARY UNITS
##XFACTOR= (AFFN)	(Factor by which the X-values in ##XYDATA= must be multiplied to obtain the original values)
##YFACTOR= (AFFN)	(Factor by which the Y-values in ##XYDATA= must be multiplied to obtain the original values)
##FIRSTX= (AFFN)	(Unscaled first X-value in ##XYDATA=)
##LASTX= (AFFN)	(Unscaled last X-value in ##XYDATA=)
##NPOINTS= (AFFN)	(Number of data points in ##XYDATA=)
##FIRSTY= (AFFN)	(Unscaled first Y-value in ##XYDATA=)
##XYDATA= (AFFN or ASDF)	(X++(Y..Y))
##END=	

Example 2. Raw data.

```

##TITLE= PFK
##JCAMP-DX= 5.00 $$ ISAS JCAMP-DX program (V.1.0)
##DATA TYPE= CONTINUOUS MASS SPECTRUM
##DATA CLASS= XYDATA
##ORIGIN= R. Fobbe, ISAS Dortmund, Germany
##OWNER= COPYRIGHT (C) 1994 by ISAS Dortmund, Germany
##SPECTROMETER/DATA SYSTEM= VG 7070E
##INSTRUMENTAL PARAMETERS= LOW RESOLUTION
##SPECTROMETER TYPE= EB
##INLET= DIRECT
##IONIZATION MODE= EI+
##ACQUISITION RANGE= 199.25, 122.50
##XUNITS= SECONDS
##YUNITS= COUNTS
##XFACTOR= 0.4271981E-03
##YFACTOR= 20998.87
##FIRSTX= 13.998
##LASTX= 6.999
##NPOINTS= 346
##FIRSTY= 9953464
##XYDATA= (X + +(Y..Y))
32767D7417J9J8j5M0M4Q1M7r7I1LL5R6r0j6lk8J9J8I4J44K5k50Oq7J25m4N018M7OJ44
31247F71j19K9R9j12J9%l8R7o9i1L06l12n3K2J96j78n3O6%L17L4Q7o5OK09k18K8J5J3
29823F15..
1€ D71 $$ checkpoint
##END=

```

Example 3. Spectral series.

```

##TITLE= GC/MS analysis of Phenol, 2-Chlorophenol, and o-Cresol
##JCAMP-DX= 5.00 $$ ISAS JCAMP-DX program (V.1.0)
##DATA TYPE= MASS SPECTRUM
##DATA CLASS= NTUPLES
##ORIGIN= H. Mayer, ISAS Dortmund, Germany
##OWNER= COPYRIGHT (C) 1994 by ISAS Dortmund, Germany
##SPECTROMETER/DATA SYSTEM= Finnigan MAT Magnum
##SPECTROMETER TYPE= TRAP
##INLET= GC
##IONIZATION MODE= EI+
##NTUPLES= MASS SPECTRUM
##VAR_NAME= MASS, INTENSITY, RETENTION TIME
##SYMBOL= X, Y, T
##VAR_TYPE= INDEPENDENT, DEPENDENT, INDEPENDENT
##VAR_FORM= AFFN, AFFN, AFFN
##VAR_DIM= , , 3
##UNITS= M/Z, RELATIVE ABUNDANCE, SECONDS
##FIRST= , , 272
##LAST= , , 333
##PAGE= T = 272
##NPOINTS= 18
##DATA TABLE= (XY..XY), PEAKS
50, 2.52; 51, 9.32; 52, 7.42; 53, 1.30; 54, 5.46; 61, 4.07
62, 5.46; 63, 11.17; 64, 2.52; 65, 39.72; 66, 63.70; 67, 4.13
68, 1.22; 77, 1.89; 79, 1.63; 93, 2.13; 94, 100.00; 95, 8.09
##PAGE= T = 301
##NPOINTS= 26
##DATA TABLE= (XY..XY), PEAKS
50, 5.84; 51, 9.55; 52, 4.19; 53, 1.12; 54, 12.67; 60, 3.80
61, 10.16; 62, 13.47; 63, 58.30; 64, 60.43; 65, 33.02; 66, 4.32
72, 1.70; 75, 1.62; 91, 1.03; 92, 24.95; 93, 4.20; 94, 1.25
99, 7.20; 100, 19.83; 101, 3.45; 102, 6.47; 128, 100.00; 129, 6.52
30, 32.45; 131, 2.13
##PAGE= T = 333
##NPOINTS= 26
##DATA TABLE= (XY..XY), PEAKS
50, 3.93; 51, 22.60; 52, 29.96; 53, 12.27; 54, 19.93; 55, 4.24
56, 3.64; 61, 3.55; 62, 5.12; 63, 14.49; 64, 2.36; 65, 4.70
56, 2.57; 68, 1.25; 76, 1.57; 77, 53.08; 78, 12.56; 79, 64.79
30, 30.92; 81, 4.33; 89, 20.26; 90, 24.82; 91, 9.30; 107, 91.80
38, 100.00; 109, 8.55
##END NTUPLES= MASS SPECTRUM
##END=

```

##END NTUPLES= (string)
##END=

MASS SPECTRUM

series can be different, it is not possible to use the JCAMP-DX Version 5.0 record ##VAR_DIM= to store this number. This means that each data page must contain its own record ##NPOINTS=. Further records which are unique to this particular spectrum (e.g., ##.BASE PEAK

INTENSITY=) can be inserted between ##PAGE= and ##NPOINTS= in the data page.

In each spectrum of the series, the Y-values in ##DATA TABLE= are normalized to the intensity of the base peak in this spectrum (Y-value of the base peak is set to 100.0).

TABLE VI. Labeled-data-records for notes.

Label (data form)	Content
\$\$ Miscellaneous	
##CLASS= (string)	(Quality of spectrum or IUPAC class of digital representation)
##DATE= (string)	(YY/MM/DD)
##TIME= (string)	(HH:MM:SS)
##SOURCE REFERENCE= (text)	(original spectrum identification)
##CROSS REFERENCE= (text)	(see section 6.1.2)
\$\$ Sample Information	
##SAMPLE DESCRIPTION= (text)	e.g., (composition) or (origin)
##CAS NAME= (string)	(CAS name)
##NAMES= (string)	e.g., (common name)
##MOLFORM= (string)	(molecular formula)
##CAS REGISTRY NO= (string)	(CAS number)
##MP= (AFFN)	(melting point in °C)
##BP= (AFFN)	(boiling point in °C)
##REFRACTIVE INDEX= (string)	e.g., ND = 1.542^20 (index at 20°C for Na D line)
##DENSITY= (AFFN)	(density in g/cm³)
##MW= (AFFN)	(molecular weight)
##CONCENTRATIONS= (string)	(NCU) (name, concentration, unit)
\$\$ Equipment	
##SPECTROMETER/DATA SYSTEM= (text)	(see section 6.1.1)
##INSTRUMENTAL PARAMETERS= (text)	(see section 6.1.1)
\$\$ Sampling Information	
##SAMPLING PROCEDURE= (text)	(mode of acquisition)
##STATE= (string)	e.g., SOLID, LIQUID or GAS
##DATA PROCESSING= (text)	(see section 6.1.1)
\$\$ Comments	
##= (text)	(comment record)
\$\$ (text)	(line comment)
##XLABEL= (text)	(label for the X-axis)
##YLABEL= (text)	(label for the Y-axis)
\$\$ Recommended Spectral Parameters	
##RESOLUTION= (string)	e.g., $m/\Delta m$ for sector field mass spectrometers
##DELTA X= (AFFN)	(nominal spacing between data points) The actual value must be calculated from (LASTX-FIRSTX)/(NPOINTS-1).

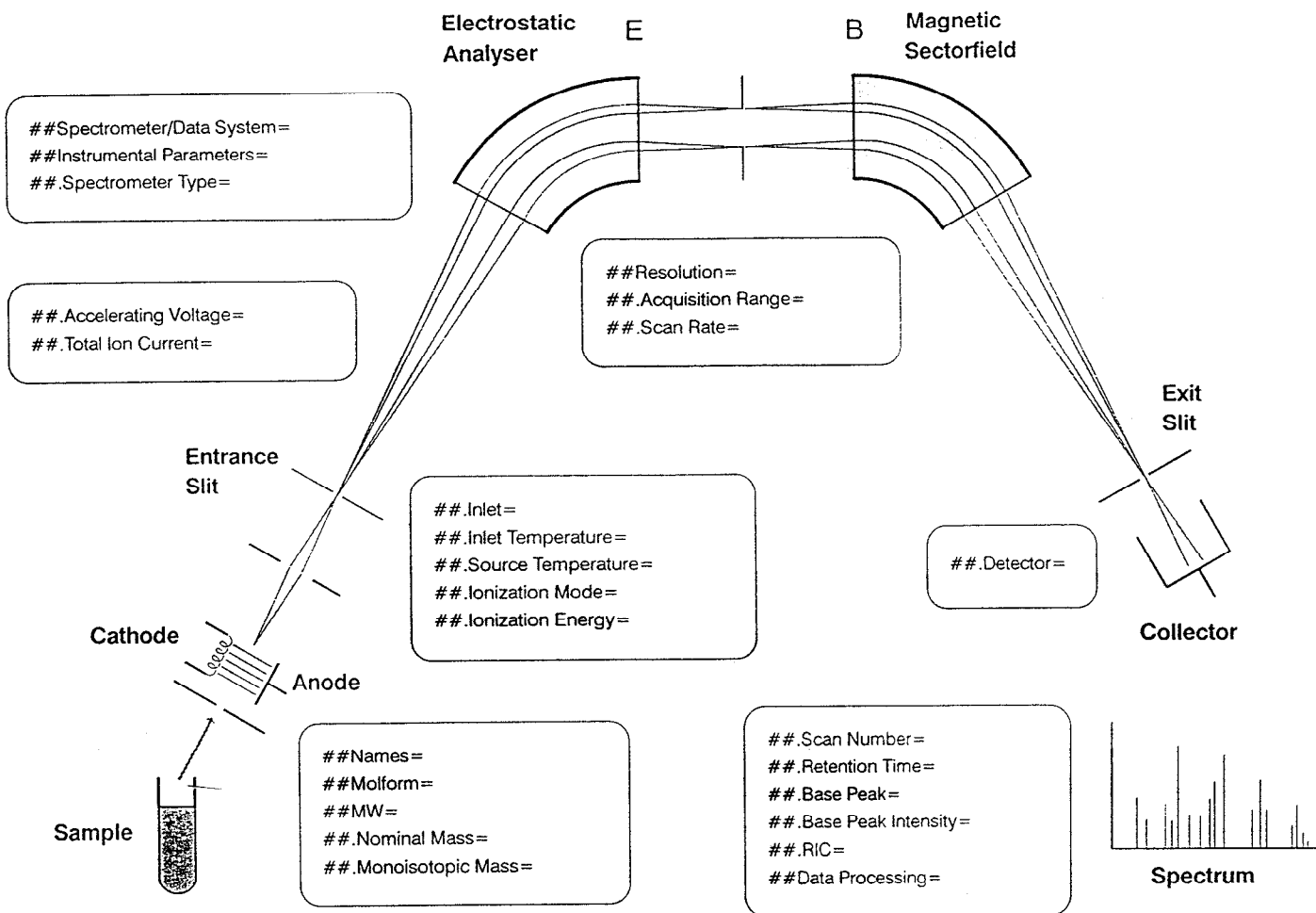


FIG. 1. An example of labeled-data-records for mass spectra.

6. THE NOTES

Notes are all records which detail the sample, the measuring instrument, the measurement parameters, or the data handling in detail. Their use is optional.

(6.1) **GLOBAL NOTES.** All notes defined in JCAMP-DX Version 4.24 are allowed in so far as they are relevant in mass spectrometry. These LDRs can be referred to in detail in Ref. 1, section 7.1, *Miscellaneous* (excepting the records **##ORIGIN=** and **##OWNER=**, which are defined with a higher priority; see 5.1.4); 7.2, *Sample Information*; 7.3, *Equipment*; and 7.4, *Sampling Information*; as well as 7.5, *Comments*, and 6.3, *Recommended Spectral Parameters*.

Table VI gives some of the allowed LDRs and how to apply them for mass spectrometry data files.

(6.1.1) Above all other records provided within the JCAMP-DX Version 4.24 protocol, the use of the records **##SPECTROMETER/DATA SYSTEM=**, **##INSTRUMENTAL PARAMETERS=**, and **##DATA PROCESSING=** are strongly recommended. Sensible text to describe the data processing could be "AVERAGE" or "BACKGROUND SUBTRACTION", for example.

(6.1.2) **##CROSS REFERENCE= (TEXT)** refers to additional spectra or structures. The format of the following example should be used (1) for data blocks stored in separate external JCAMP-DX files or (2) for compound JCAMP-DX files where some spectra or structure blocks

belong to the same file and each block has a unique **##BLOCK_ID=**:

```
##CROSS REFERENCE= NMR SPECTRUM: EXTERNAL_FILE= FILE1234.DX
STRUCTURE: BLOCK_ID= 1
INFRARED SPECTRUM: BLOCK_ID= 2"
```

(6.2) **MASS SPECTROMETRY SPECIFIC NOTES.** The following record definitions are optional (See Fig. 1).

(6.2.1) **##.INLET TEMPERATURE= (AFFN).** Inlet temperature in °C.

(6.2.2) **##.SOURCE TEMPERATURE= (AFFN).** Source temperature in °C.

(6.2.3) **##.IONIZATION ENERGY= (AFFN).** Ionization energy in eV.

(6.2.4) **##.ACCELERATING VOLTAGE= (AFFN).** Accelerating voltage in volts.

(6.2.5) **##.TOTAL ION CURRENT= (AFFN, string).** The total ion current as measured with the units of measurement. The strings "COUNTS" and "VOLTS" are defined for the units of measurement. The record must *not* be used to store the reconstructed ion current (RIC).

(6.2.6) **##.ACQUISITION RANGE= (AFFN, AFFN).** The measurement region in amu (first, last).

(6.2.7) **##.SCAN RATE= (AFFN, string).** Scan rate in "SECONDS/DECADE" or "MASSES/SECOND" with the unit of measurement as defined.

(6.2.8) **##.DETECTOR= (Text).** Type of detector.

(6.2.9) **##.SCAN NUMBER= (AFFN)**. Scan number.
(6.2.10) **##.RETENTION TIME= (AFFN)**. Retention time in seconds.

(6.2.11) **##.BASE PEAK= (AFFN)**. Position of the base peak in XUNITS.

(6.2.12) **##.BASE PEAK INTENSITY= (AFFN, string)**. Unscaled Y-value of the base peak in "COUNTS" or "VOLTS" with the units of measurement as defined.

(6.2.13) **##.RIC= (AFFN)**. Reconstructed ion current in counts.

(6.2.14) **##.NOMINAL MASS= (AFFN)**. Nominal mass of the molecule. This integer value and the following LDR (6.2.15) are to be differentiated from the standard value in chemistry of the relative molecular mass averaged over all isotopes (**##MW=**).

(6.2.15) **##.MONOISOTOPIC MASS= (AFFN)**. Mass of the most common isotope peak in amu.

ACKNOWLEDGMENTS

The authors would like to thank Dr. Peter Hoever (Bayer AG) for stimulating discussions and Robert S. McDonald, PhD., for numerous helpful hints. This work was partially financed by the Bundesminister für Forschung und Technologie, as well as the Ministerium für Wissenschaft und Forschung of Nordrhein-Westfalen, Germany.

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