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JCAMP-DX. A STANDARD FORMAT FOR THE EXCHANGE OF ION MOBILITY SPECTROMETRY DATA

(IUPAC Recommendations 2001)

Prepared for publication by
JÖRG INGO BAUMBACH[‡], ANTONY N. DAVIES[1], PETER LAMPEN, AND HARTWIG SCHMIDT

ISAS, Institut für Spektrochemie und Angewandte Spektroskopie, Bunsen-Kirchhoff-Strasse 11, 44139 Dortmund, Germany

[‡]Corresponding author
[1]Current address c/o CREON•LAB•CONTROL AG, Europaallee, 27-29 50226 Frechen, Germany

JCAMP-DX. A standard format for the exchange of ion mobility spectrometry data

(IUPAC Recommendations 2001)

Abstract: The relatively young field of ion mobility spectrometry has now advanced to the stage where the need to reliably exchange the spectroscopic data obtained worldwide by this technique has become extremely urgent. To assist in the validation of the various new spectrometer designs and to assist in inter-comparisons between different laboratories reference data collections are being established for which an internationally recognized electronic data exchange format is essential.

To make the data exchange between users and system administration possible, it is important to define a file format specially made for the requirements of ion mobility spectrometry. The format should be computer readable and flexible enough for extensive comments to be included. In this document, we define a data exchange format, agreed on by a working group of the International Society for Ion Mobility Spectrometry at Hilton Head Island, USA (1998) and Buxton, UK (1999).

This definition of this format is based on the IUPAC JCAMP-DX protocols, which were developed for the exchange of infrared spectra [1] and extended to chemical structures [2], nuclear magnetic resonance data [3], and mass spectra [4]. This standard of the **J**oint **C**ommittee on **A**tomic and **M**olecular **P**hysical Data is of a flexible design. The International Union of Pure and Applied Chemistry have taken over the support and development of these standards and recently brought out an extension to cover year 2000 compatible date strings and good laboratory practice [5]. The aim of this paper is to adapt JCAMP-DX to the special requirements of ion mobility spectra [6].

1. INTRODUCTION

JCAMP-DX is an electronic file-based format using ASCII characters (**A**merican **S**tandard **C**ode of **I**nformation **I**nterchanging) reduced to the printable character. This guarantees the acceptance on all computer systems. The main components to describe the ion mobility spectrometer (IMS) and the spectra are shown in Fig. 1.
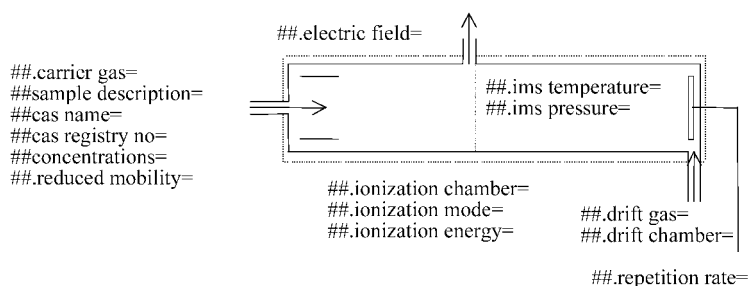

Fig. 1 The main ion mobility spectrometry specific and generic terms to be stored in a JCAMP-DX data file are shown here.

2. DEFINITIONS

The following definitions are important for the understanding of the JCAMP-DX protocol.

2.1 Labeled-data-records

Labeled-data-records (LDRs) consist of a flagged *data-label* and an associated *data-set*. An LDR begins with a *data-label-flag* (##) and ends with the next data-label-flag. LDRs are divided into lines of 80 or fewer characters, terminated by <CRLF>. End-of-line is equivalent to a blank, except for certain special cases. Each LDR occupies as many lines as necessary. A data-label is the name of an LDR. It is delimited by a data-label-flag (##) and a *data-label-terminator* (=), for example ##TITLE= is a data-label for the definition of the working title of the following spectrum. A line contains no more than one data-label. When labels are parsed, alphabetic characters are converted to upper case, and all spaces, dashes, slashes, and underlines are discarded. Thus, XUNITS and X-units are equivalent.

There are two kinds of LDR: core and note. Core LDRs are required. Notes are optional. Every definition of an LDR should include if it is a core or a note.

In Sections 2.2–2.5, we discuss the forms used for defined data-sets.

2.2 Text

The LDRs contain descriptive information for humans, not normally intended to be parsed by computers, i.e., title, comments, origin, etc.

2.3 String

Some LDRs contain predefined text fields intended to be parsed by computers and read by humans. The format of each string field is specified under the LDR in which it is used.

2.4 AFFN

The easiest way to write the data is to use the ASCII free format numeric. This format is important to simplify direct user input. It is a format similar to freeform input in BASIC. A field starts either with +, –, decimal point, or digit. E is the only allowed character to give the power of 10 by which the field must be multiplied. It is followed by + or – and two or three digits. The numeric field is terminated either by E, comma, or blank.

2.5 ASDF

This is the ASCII squeezed difference form. The LDRs contain tabular data using JCAMP-DX data compression scheme (see Section 3.4.1).

2.6 Comments

Comments may be specified by a data-label-flag plus a data-label-terminator, with a null data-label (##=). Such comments may continue for more than one line, terminating at the next data-label-flag.

Comments may be entered at any point in a line by prefixing the first word of the comment by $$. Such comments continue only to the end of the current line, and they do not terminate an LDR.

3. CORE

This section describes the data labels for the JCAMP-DX core data.

The core consists of four parts. The first part, called the *fixed header information*, contains generic LDRs, which are required for all JCAMP-DX files and which appear at the beginning of each file in a given order. The *variable header information* contains records that are data-type-specific (in this case IMS specific) or that are only used in special types of JCAMP-DX files (e.g., compound files). Whether a particular is required or not depends on the application. The third section, *core data*, contains the relevant parameters for the fourth section, the *data table*. The type of data in the data table determines the parameters that must appear in the core data. Only one data table may appear per JCAMP-DX block (a block being a part of the JCAMP-DX file starting with ##TITLE= and ending with ##END=).

3.1 Core fixed header information

3.1.1 ##TITLE= (TEXT)
Title and/or reason of the measurement.
　　(*Required*)

3.1.2 ##JCAMP-DX= (STRING)
The version number of this protocol is 5.01. A description of the software used to generate the file follows the version number as a comment.

　　For example:
　　##JCAMP-DX= 5.01　　$$ JCAMP-DX for IMS (NT4 version 1.0 ISAS Germany)
　　(*Required*)

3.1.3 ##DATA TYPE=　(STRING)
Keywords:
　　ION MOBILITY SPECTRUM or
　　IMS PEAK TABLE or
　　IMS PEAK ASSIGNMENTS or
　　LINK

　　Distinguishes between different kinds of spectra such as IMS-, NMR-, or IR-data. The string ION MOBILITY SPECTRUM reports a continuous spectrum located at the ##XYDATA= LDR, and IMS PEAK ASSIGNMENTS reports distinct and analyzed peaks located in the ##PEAK ASSIGNMENTS= LDR.
　　(*Required*)

3.1.4 ##DATA CLASS= (STRING)
Keywords:
　　XYDATA or
　　XYPOINTS or
　　PEAK TABLE or
　　ASSIGNMENTS

　　This label defines the type of tabular data within the data block and is not to be used for link blocks.
　　(*Required*)

3.1.5 ##ORIGIN= (TEXT)
Here, the name of organization, address, telephone number, name of individual contributor, email, etc., as appropriate must be added. This information is not optional.
　　(*Required*)

3.1.6 ##OWNER= (TEXT)

It is possible to set here a copyright linked to the spectrum, that has the form: "COPYRIGHT (C) <year> by <name>". If ##OWNER= contains "PUBLIC DOMAIN", the implication is that the data may be copied without permission on the authority of whoever is named under ##ORIGIN=

(*Required*)

3.1.7 ##END=

It is important to have a mark at the end of file in the data format to know that transfer has been complete and to distinguish between the blocks of a multi-spectrum file.

(*Required*)

3.2 Core variable header information

The JCAMP-DX standard is easy to understand and expand. Many LDRs are already defined in previous JCAMP-DX protocols, and they should be used for ion mobility spectrometry. However, in the case of the equipment parameters, the particular requirements of this technique call for some special LDRs. Data-type-specific LDRs start with "##." (see Section 4.2). In the following part, definitions are given for LDRs that will allow a precise description of the equipment parameters.

3.2.1 ##BLOCKS= (AFFN) and ##BLOCK_ID= (AFFN)

Blocks are used as suggested in the JCAMP-DX 4.24 protocol (3.2) [1] with the extensions defined in the JCAMP-CS protocol (5.13) [2] to provide inter-block referencing.

For ease of use, it is recommended to use separate files and to avoid the use of blocks. However, when, for example, XYDATA and a PEAK TABLE must be stored in the same file, these must be written as a compound file [1]. The use of compound data files is, of course, optional but when more than one block per file is stored the ##BLOCKS= LDR has the priority REQUIRED.

A compound JCAMP-DX file consists of a LINK block (##DATA TYPE=LINK) surrounding the DATA blocks, and the total number of DATA blocks (N) must appear in the LINK block header (##BLOCKS=N). A unique positive integer (n) should be assigned to each DATA block inside the compound file (##BLOCK_ID=n). Linking of the blocks can then be achieved using ##CROSS REFERENCE= (see Example). These records are to be used in compound JCAMP-DX files to provide inter-block referencing.

(*Required only for compound files*)

EXAMPLE

```
##TITLE= example compound data file          $$ title of the whole compound file
##JCAMP-DX= 5.01                             $$ name & version no. of JCAMP-DX
                                                software

##DATA TYPE= LINK
##BLOCKS= 2                                  $$ number of data blocks
##ORIGIN=                                    $$ name of contributor, organization,
                                                address, telephone, etc.

##OWNER=                                     $$ COPYRIGHT (C)'year' by 'name'
                                                or PUBLIC DOMAIN

##TITLE=                                     $$ title of the first data block
##JCAMP-DX= 5.01
##DATA TYPE= ION MOBILITY SPECTRUM
##DATA CLASS= XYDATA
##BLOCK_ID= 1
##ORIGIN=                                    $$ name of contributor, organization,
                                                address, telephone etc.
```

```
##OWNER=                                    $$ COPYRIGHT (C)'year' by 'name'
                                               or PUBLIC DOMAIN
##CROSS REFERENCE= IMS PEAK TABLE:BLOCK_ID=2
. . .
##END=                                      $$ end of first data block
##TITLE=                                    $$ title of the second data block
##JCAMP-DX= 5.01
##DATA TYPE= IMS PEAK TABLE
##DATA CLASS= PEAK TABLE
##BLOCK_ID= 2
##ORIGIN=                                   $$ name of contributor, organization,
                                               address, telephone etc.
##OWNER=                                    $$ COPYRIGHT (C)'year' by 'name'
                                               or PUBLIC DOMAIN
##CROSS REFERENCE= ION MOBILITY SPECTRUM: BLOCK_ID=1
. . .
##END=                                      $$ end of second data block
##END=                                      $$ end of link block and file
```

3.2.2 ##.IMS PRESSURE= (AFFN)
Pressure inside the IMS system in kilopascal.
>(*Required*)

3.2.3 ##.CARRIER GAS= (TEXT)
A description of the carrier gas is given here.
>(*Required*)

3.2.4 ##.DRIFT GAS= (TEXT)
A description of the drift gas is required when used in addition to the carrier gas**.**
>(*Required*)

3.2.5 ##.ELECTRIC FIELD= (AFFN, AFFN)
The electric field description is divided in two parts: The field in the ionization chamber and the one in the drift chamber (in volt/centimeter) separated by commas, including the polarity (+ for positive ions detected and – for negative ions, respectively).
>(*Required*)

3.2.6 ##.ION POLARITY= (STRING)
The polarity of the measured ions. Allowed values are POSITIVE or NEGATIVE.
>(*Required*)

3.2.7 ##.IONIZATION MODE= (STRING)
The following keywords define how the system ionizes the gas:

UV	ultraviolet source
BR	beta radiation source
AL	alpha radiation source
PD	partial discharge
CD	corona discharge
ESI	electrospray ionization
LI	laser ionization
LD	laser desorption
SI	surface ionization
SY	synchrotron radiation

For more detailed information, it is possible to give a comment such as $$ ^63Ni source. (*Required*)

3.2.8 ##.IMS TEMPERATURE= (AFFN[, AFFN])

Here, the first value is characterizing the temperature in the drift chamber, the second value is characterizing the temperature in the ionization chamber in °C. The second value is optional and separated by a comma.

(*Required*)

3.2.9 ##.SHUTTER OPENING TIME= (AFFN)

Shutter opening time in microseconds.

Without knowing the time the shutter was open, it is not possible to calculate the individual mobilities.

(*Required*)

3.3 Core data

3.3.1 ##XUNITS= (STRING) and ##YUNITS= (STRING)

Here, the units of the axes can be given. The following keywords are defined:

For ##XUNITS=: SECONDS, MILLISECONDS, MICROSECONDS, and NANOSECONDS.
For ##YUNITS=: MICROAMPERES, NANOAMPERES, and PICOAMPERES.
(*Required*)

3.3.2 ##FIRSTX= (AFFN) and ##LASTX= (AFFN)

First and last actual abscissa values of ##XYDATA=. First tabulated abscissa times ##XFACTOR= should equal ##FIRSTX=.

(*Required for ##DATA CLASS=XYDATA*)

3.3.3 ##FIRSTY= (AFFN)

Here, the actual ordinate value corresponding to ##FIRSTX= is meant. ##FIRSTY= should be equal ##YFACTOR= times the first Y-value in ##XYDATA=.

(*Required for ##DATA CLASS=XYDATA*)

3.3.4 ##XFACTOR= (AFFN) and ##YFACTOR= (AFFN)

The values of a spectrum may be converted to integer to save space and allow the DIFDUP format (see Section 3.4.1). It is important to select a convenient scaling to keep the file within reasonable limits, but to store all significant digits. In such a case, the ##XFACTOR= and ##YFACTOR= LDR contain a floating-point number to be multiplied by the values in ##XYDATA= to arrive at the original data point value.

In most cases, ±32767 is sufficient, therefore this is the *recommended ordinate scaling*. If a larger scaling is necessary, it is required to give the actual unscaled maximum and minimum of the ordinates in the records ##MAXY= and ##MINY=. This avoids a 2-byte integer overflow in the program reading the data table.

For example, if a Y-value with 9 significant figures (e.g., 0.002457194) needs to be converted to an integer value for ASDF coding then:

a)   divide by the maximum of the absolute Y-value (say, 0.346299765),
b)   multiply by the largest integer value (MAXINT) necessary to place all significant figures left of the decimal point, and
c)   convert to integers.

For this example:

$Y_{integer}$ $=INTEGER((Y_{real} / MAX(ABS(Y_{real})))*MAXINT)$
$=INTEGER(0.002457194/0.346299765)*1.0E+11$
$=INTEGER(709556935.4487)$
$=709556935$
then $\#\#YFACTOR= (MAX(ABS(Y_{real})))/MAXINT$
    (*Required for ##DATA CLASS=XYDATA*)

3.3.5 ##NPOINTS= (AFFN)
The number of points in the data table is required for all data classes: XYDATA, XYPOINTS, PEAK TABLE, and ASSIGNMENTS.
    (*Required*)

3.4 Core data table

Data must be stored in one of the following data formats (Sections 3.4.1–3.4.4). Only one of these formats is allowed per DATA block, and the selected data table is given in the header, e.g., ##DATA CLASS=XYDATA.

3.4.1 ##XYDATA= (AFFN or ASDF).
This LDR contains a table of spectral data with abscissa values at equal intervals specified by parameters defined in Section 3.3. The label is followed by a *variable list*, (X++(Y..Y)) where .. indicates indefinite repeat of Y-values until the end of line and ++ indicates that X is incremented by (LASTX-FIRSTX) / (NPOINTS-1) between two Y-values. For discrete point, the AFFN form is allowed where each Y value is written out in full. This form creates large files, but is easily human-readable. The following ASDF forms produce smaller files at the cost of reduced human readability.

SQUEEZED FORM (SQZ)
Data compression is possible using the squeezed form (SQZ) in which the delimiter, the leading digit, and sign are replaced by a pseudo-digit from Table 1.
    For example, the Y-values 30, 32 would be represented as C0C2.

DIFFERENCE FORM (DIF)
For a better compression, it is possible to use the *difference form* (DIF) where the delimiter, leading digit, and sign of the difference between adjacent values are transformed in a pseudo-digit from Table 1.
    For example, the Y-values 30, 32 would now be represented as C0K.
    To ensure data coding is correct, a Y-value check is built-in. Each line starts with the absolute X- and Y-value, which is the same as the last calculated value of the previous line. The last line of a block of DIF data contains only the abscissa and ordinate for a Y-value check of the last ordinate.

DUPLICATE SUPPRESION (DUP)
Another possible variation is to include *duplicate suppression* (DUP), replacing two or more adjacent and identical numbers with pseudo-digits as given in Table 1. This can be used with all ASDF forms.

Table 1 Pseudo-digits used to compress spectra data in SQZ-, DIF-, and DUP-format.

ASCII digits	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
DUP		S	T	U	V	W	X	Y	Z	s

For example, 50 50 50 50 becomes E0V when combining DUP with SQZ.

The best compression (but the least human-readable form) can be achieved when DIF and DUP are combined to provide the form called DIFDUP. In this format, the duplicate count is obtained by counting identical differences.

The example above becomes E0%%% in DIF form and E0%U in DIFDUP form.

Example for uncompressed data storage:

```
##TITLE= Incomplete example file for uncompressed data!

..........
##XUNITS= MILLISECONDS
##YUNITS= NANOAMPERES
##XFACTOR= 1
##YFACTOR= 0.1
##FIRSTX= 4
##LASTX= 56
##NPOINTS= 53
##FIRSTY= 0
##XYDATA= (X++(Y..Y)
4 0 0 0 0 2 4 4 4 7
13 5 4 4 5 5 7 10 11 11
22 6 5 7 6 9 9 7 10 10
31 9 10 11 12 15 16 16 14 17
40 38 38 35 38 42 47 54 59 66
49 75 78 88 96 104 110 121 128
##END=
```

Example for DIFDUP-form:

```
##TITLE= Incomplete example file for DIFDUP data form!

......
##XUNITS= MILLISECONDS
##YUNITS= NANOAMPERES
##XFACTOR= 1
##YFACTOR= 0.1
##FIRSTX= 4
##LASTX= 56
##NPOINTS= 53
##FIRSTY= 0
##XYDATA= (X++(Y..Y)
4@VKT%TLkj%J%KLJ%njKjL%kL%jJULJ%kLK1%lLMNPNPRLJ0QTOJ1P
56A28
##END=
```

3.4.2 ##XYPOINTS= (AFFN)

This LDR contains a table of spectral data with unequal abscissa increments. The label is followed by a variable list, (XY..XY). X and Y are separated by commas, data pairs are separated by semicolons or blanks. This LDR should not be used for peak tables.

3.4.3 ##PEAK TABLE= (AFFN)

It is recommended to store peak information using ##PEAK ASSIGNMENTS=, however, for backward compatibility this definition is included. This data table contains a table of peaks where the peak data starts on the following line. The label is followed by the variable list (XY) or (XYW) for peak position, intensity, and width, where known, on the same line. The function used to calculate the peak width

should be defined by a $$ comment in the line below the label. The peak groups are separated by a semi-colon or space, components of a group are separated by commas.

3.4.4 ##PEAK ASSIGNMENTS= (STRING)

Variable list: (XA), (XYA), or (XYWA)

After this LDR, a list of peaks and their assignments for each components are given in the following form:

$(X_1[, Y_1][, W_1], <A_1>)$

. . . .

$(X_i[, Y_i][, W_i], <A_i>)$

X and Y indicate the location and height of each peak in units given by ##XUNITS= and ##YUNITS=. W stands for width in ##XUNITS=, and A represents a string describing the assignment enclosed in angle brackets.

The parentheses provide a start and end flag of each assignment. Square brackets indicate optional information. It is important for the technical readability to have the same format for the whole peak assignment table and describe it after the ##PEAK ASSIGNMENTS= LDR with (XA), (XYA), or (XYWA). This LDR should be followed by a comment, which gives the method of finding the peak.

For example:

```
##PEAK ASSIGNMENTS= (XYWA)
(15, 20.0, 1.0,<benzene>)
(30, 40.0, 2.0,<toluene>)
......
```

4. NOTES

The notes portion of a JCAMP-DX file or block complements the core. Notes describe an experiment in greater detail than does ##TITLE=, including descriptions of equipment, method of observation, and data processing, as appropriate. Notes may contain information, which is not found in the native file in which data is originally collected by an instrument. Notes are placed before the core data section to permit them to be viewed without listing the whole file. The contents of the notes depend on the user as well as the technique or application. Notes will vary for different samples, sites, data systems, and applications.

4.1 Global notes

These have been already defined in JCAMP-DX and are common to all spectroscopy types. The file headers, spectral and sample parameters are often the same for different analytical techniques. This allows us to implement many of the standard LDRs from the existing JCAMP-DX protocols. The list given below is only a selection from those allowed. A complete list can be found in the references [1–5].

At least one of the optional LDRs described in Sections 4.1.4–4.1.8 should be included in each JCAMP-DX file. This is important for later archiving, as these fields will yield more detailed information on the content of the data stored than a simple ##TITLE= field.

4.1.1 ##LONG DATE= (STRING)

Date of measurement is required by many agencies and recommended in the year 2000 form: YYYY/MM/DD [HH:MM:SS[.SSS] [±XXXX]]. YYYY is the long format of the year, MM the number of the month, DD the number of the day, HH the hour, MM the minutes, SS.SSS the seconds and fractions of a second of the measurement, ±XXXX is the difference to the UTC (e.g., +0100 is one hour difference to UTC).

(*Optional*)

4.1.2 ##SOURCE REFERENCE= (TEXT)

Here, an identification of the original spectrum file in native format or library name and serial number is possible, for example.

(*Optional*)

4.1.3 ##CROSS REFERENCE= (TEXT)

Used to link additional data for the same sample, such as other types of spectra or chemical structures, for example:

    ##CROSS REFERENCE=
    ION MOBILITY SPECTRUM: EXTERNAL_FILE= FILENAME.DX
    IMS PEAK TABLE: BLOCK_ID=16
    STRUCTURE: BLOCK_ID=4

    ......
(*Optional*)

4.1.4 ##SAMPLE DESCRIPTION= (TEXT)

If the sample is not a pure compound, this field should contain its description, i.e., composition, origin, appearance, results of interpretation, etc. If the sample is a known compound, the following LDRs specify structure and properties, as appropriate.

(*Optional*)

4.1.5 ##CAS NAME= (STRING)

Name according to Chemical Abstracts naming conventions as described in the CAS Index Guide is required here. Examples can be found in Chemical Abstracts indices or the Merck Index. Greek letters are spelled out, and standard ASCII capitals are used for small capitals, Sub- and superscripts are indicated by prefixes / and ∧. Example: alpha-D-glucopyranose, 1-(dihydrogen phosphate).

(*Optional*)

4.1.6 ##NAMES= (STRING)

Here, the common, trade, or other names are allowed. Multiple names are placed on separate lines.

(*Optional*)

4.1.7 ##MOLFORM= (STRING)

Another possibility of describing the sample is to write down the molecular formula. Elemental symbols are arranged with carbon first, followed by hydrogen, and then remaining element symbols in alphabetic order.

The first letter of each elemental symbol is capitalized. The second letter, if present, is lower case. One-letter symbols must be separated from the next symbol by a blank or digit. Sub- and superscripts are indicated by the prefixes: / and ∧, respectively. Sub- and superscripts are terminated by the next nondigit. Slash may be omitted for subscripts.

For readability, each atomic symbol may be separated from its predecessor by a space. For substances that are represented by dot disconnected formulas (hydrates, etc.), each fragment is represented in the above order, and the dot is represented by *. Isotopic mass is specified by a leading superscript. D and T may be used for deuterium and tritium.

(*Optional*)

Examples:

    C2H4O2 or C2 H4 O2   (acetic acid)
    H2 ∧17O   (water, mass 17 oxygen)

4.1.8 ##CONCENTRATIONS= (STRING)

The list of the known components and their concentrations has the following form, where N stands for the name and C for the concentration of each component in units given with U in the form:

##CONCENTRATIONS= (NCU)

(N_1, C_1, U_1)

   . . .

(N_i, C_i, U_i)

The group for each component is enclosed in parentheses. Each group starts a new line and may continue on following lines.

(*Optional in JCAMP-DX, but in this case strongly recommended*)

4.1.9 ##SPECTROMETER/DATA SYSTEM= (TEXT)

This LDR contains manufacturers' name, model of spectrometer, software system, and release number, as appropriate in the form used by the manufacturer.

(*Optional*)

4.1.10 ##DATA PROCESSING= (TEXT)

Here, all mathematical procedures used before storing the data in the JCAMP-DX file are described. This LDR is also important in peak assignments.

(*Optional*)

4.1.11 ##XLABEL= (TEXT) and ##YLABEL= (TEXT)

These LDRs give the possibility of labeling the axes.

(*Optional*)

4.1.12 ##MAXX= (AFFN), ##MINX= (AFFN), ##MAXY= (AFFN), and ##MINY= (AFFN)

These LDRs give the largest and smallest actual X- and Y-values in a spectrum. ##MAXY= and ##MINY= are required if Y-range exceeds recommended ordinate scaling (Section 3.3.4).

(*Optional*)

4.2 Data-type-specific notes

Data-type-specific labels are RESERVED labels that are defined by qualified user groups for a particular data-type. A data-type-specific label is distinguished by a *data-type-specific label name* which starts with a period (e.g., ##●REDUCED MOBILITY=). Choice of period as distinguishing character is by analogy with the convention for data-structure names in Pascal and C. Effectively, the full label name is the concatenation of the data-type name and the label-name, with a period in between, i.e., ##ION MOBILITY SPECTRUM●REDUCED MOBILITY=.

4.2.1 ##.REDUCED MOBILITY= (STRING)

This LDR contains a list of reduced mobilities and their assignments for each of the components, where K_0 is the reduced mobility and A is a string describing the assignment in closed angle brackets in the form:

(K_{01}, <A_1>)

(K_{02}, <A_2>)

....

(K_{0i}, <A_i>)

where the K_0 values are the known reduced mobilities in $cm^2\ V^{-1}\ s^{-1}$ given according to the formula:

$$K_0 = K \cdot \frac{P \cdot T_0}{P_0 \cdot T}$$

where K is the measured mobility at pressure P and temperature T. P_0 is 101325 Pa, and T_0 is 273 K. The variable list (KA) *must* be given in the labeled-data-record and followed on the next line by the list of reduced mobilities each on its own line as shown in the example below:

##.REDUCED MOBILITY=(KA)
(2.38, <tetrachloroethene>)
(2.27, <tetrachloroethene>)
(2.06, <tetrachloroethene>)
(1.83, <tetrachloroethene>)
....
(*Optional*)

4.2.2 ##.IONIZATION ENERGY= (AFFN)
The ionization energy in eV.
(*Optional*)

4.2.3 ##.IONIZATION CHAMBER= (STRING, AFFN, AFFN[, AFFN])
and

4.2.4 ##.DRIFT CHAMBER= (STRING, AFFN, AFFN[, AFFN])
Different geometrical parameters of the ionization or drift chamber are distinguished by the following keywords:

RECT This means a rectangular chamber. It is followed by the size of the three dimensions length, width, and height in mm.

CYL Stands for a cylindrical form of the chamber. It is followed by its length and radius in mm.

(*Optional*)

4.2.5 ##.CARRIER GAS FLOW= (AFFN[, AFFN])
This LDR is divided in two flow values. The first value is linked to the ionization chamber, the second is optional, if applied. All values have the unit litre/minute.
(*Optional*)

4.2.6 ##.DRIFT GAS FLOW= (AFFN)
This LDR defines the drift gas flow into the drift chamber when a separate gas is used here to the carrier gas. All values have the unit litre/minute.
(*Optional*)

4.2.7 ##.CARRIER GAS MOISTURE= (AFFN)
The water concentration in the carrier gas is relevant to the different ionization processes. It is strongly recommended that this value be reported. This is labeled volume fraction with the units parts per million (ppm).
(*Optional*)

4.2.8 ##.IONIZATION SOURCE= (TEXT)
A description of the relevant ionization source details.

For partial discharges (##.ionization mode=PD), this would include, for example, the materials used in the construction of the source and the needle/plate gap in the form;

##.IONIZATION SOURCE= Partial Discharge: Needle = Steel, Plate = Silver, Gap = 5 mm, Potential difference = 5000 V

or for an ultraviolet lamp as source, the energy and the lamp mounting position (on or off axis);

##.IONIZATION SOURCE= UV Lamp: 10.6 eV, off-axis

or for a radioactive source, the type nature and intensity, such as

##. IONIZATION SOURCE= ^{63}Ni, 555 MBq

or

##. IONIZATION SOURCE= ^3H, 150 kBq

for laser ionization, the type of laser used, the wavelength selected and any relevant pulse information in the form

##. IONIZATION SOURCE= Nd:YAG laser, 266 nm, pulse energy 10 mJ, pulse width 30 ps

(*Optional*)

4.2.9 ##.SHUTTER GRID POTENTIAL= (AFFN)

The potential difference between the wires of the shutter in volts.

For example:

##.SHUTTER GRID POTENTIAL= 100

(*Optional*)

4.2.10 ##.REPETITION RATE= (AFFN)

The time between subsequent shutter openings in milliseconds.

For example:

##.REPETITION RATE= 100

(*Optional*)

4.2.11 ##.AVERAGES= (AFFN)

Number of transients averaged.

For example:

##.AVERAGES= 30

(*Optional*)

5. SUMMARY

The following tables list the LDRs discussed with their basic parameters shown.

<u>THE CORE</u>

Core Fixed Header Information

LDR	Data-form	Keyword	Status	Location
##TITLE=	(TEXT)		Required	3.1.1
##JCAMP-DX=	(STRING)	5.01	Required	3.1.2
##DATA TYPE=	(STRING)	ION MOBILITY SPECTRUM, IMS PEAK TABLE, IMS PEAK ASSIGNMENTS or LINK	Required	3.1.3
##DATA CLASS=	(STRING)	XYDATA, XYPOINTS, PEAK TABLE, or ASSIGNMENTS	Required	3.1.4
##ORIGIN=	(TEXT)		Required	3.1.5
##OWNER=	(TEXT)		Required	3.1.6
##END=			Required	3.1.7

Core Variable Header Information

LDR	Data-form	Keyword	Status	Location
##BLOCKS=	(AFFN)		Required for compound files	3.2.1
##BLOCK_ID=	(AFFN)		Required for compound files	3.2.1
##.IMS PRESSURE=	(AFFN)		Required	3.2.2
##.CARRIER GAS=	(TEXT)		Required	3.2.3
##.DRIFT GAS=	(TEXT)		Required	3.2.4
##.ELECTRIC FIELD=	(AFFN, AFFN)		Required	3.2.5
##.ION POLARITY=	(STRING)	POSITIVE or NEGATIVE	Required	3.2.6
##.IONIZATION MODE=	(STRING)	UV, BR, AL, PD, CD, ESI, LI, LD, SY, SI	Required	3.2.7
##.IMS TEMPERATURE=	(AFFN[,AFFN])		Required	3.2.8
##.SHUTTER OPENING TIME=	(AFFN)		Required	3.2.9

Core Data

LDR	Data-form	Keyword	Status	Location
##XUNITS=	(STRING)	SECONDS, MILLISECONDS, MICROSECONDS, NANOSECONDS	Required	3.3.1
##YUNITS=	(STRING)	MICROAMPERES, NANOAMPERES, PICOAMPERES	Required	3.3.1
##FIRSTX=	(AFFN)		Required for ##DATA CLASS= XYDATA	3.3.2
##LASTX=	(AFFN)		Required for ##DATA CLASS= XYDATA	
##FIRSTY=	(AFFN)		Required for ##DATA CLASS= XYDATA	3.3.3
##XFACTOR=	(AFFN)		Required for ##DATA CLASS= XYDATA	3.3.4
##YFACTOR=	(AFFN)		Required for ##DATA CLASS= XYDATA	3.3.4
##NPOINTS=	(AFFN)		Required	3.3.5

Core Data Table

LDR	Data-form	Keyword	Status	Location
##XYDATA=	(AFFN or ASDF)	(X++(Y..Y))		3.4.1
##XYPOINTS=	(AFFN)	(XY..XY)		3.4.2
##PEAK TABLE=	(AFFN)	(XY) or (XYW)		3.4.3
##PEAK ASSIGNMENTS=	(STRING)	(XA), (XYA) or (XYWA)		3.4.4

THE NOTES

Global Notes

LDR	Data-form	Keyword	Status	Location
##LONG DATE=	(STRING)		Optional	4.1.1
##SOURCE REFERENCE=	(TEXT)		Optional	4.1.2
##CROSS REFERENCE=	(TEXT)		Optional	4.1.3
##SAMPLE DESCRIPTION=	(TEXT)		Optional	4.1.4
##CAS NAME=	(STRING)	Names defined by CAS Index Guide	Optional	4.1.5
##NAMES=	(STRING)		Optional	4.1.6
##MOLFORM=	(STRING)		Optional	4.1.7
##CONCENTRATIONS=	(STRING)	(NCU)	Optional, but strongly recommended	4.1.8
##SPECTROMETER/ DATA SYSTEM=	(TEXT)		Optional	4.1.9
##DATA PROCESSING=	(TEXT)		Optional	4.1.10
##XLABEL=	(TEXT)		Optional	4.1.11
##YLABEL=	(TEXT)		Optional	4.1.11
##MAXX=	(AFFN)		Optional	4.1.12
##MINX=	(AFFN)		Optional	4.1.12
##MAXY=	(AFFN)		Required if Y-range exceeds recommended ordinate scaling	4.1.12
##MINY=	(AFFN)		Required if Y-range exceeds recommended ordinate scaling	4.1.12

Data-Type Specific Notes

LDR	Data-form	Keyword	Status	Location
##.REDUCED MOBILITY=	(STRING)	(KA)	Optional	4.2.1
##.IONIZATION ENERGY=	(AFFN)		Optional	4.2.2
##.IONIZATION CHAMBER=	(STRING, AFFN, AFFN[, AFFN])	RECT or CYL	Optional	4.2.3
##.DRIFT CHAMBER=	(STRING, AFFN, AFFN[, AFFN])	RECT or CYL	Optional	4.2.4
##.CARRIER GAS FLOW=	(AFFN[, AFFN])		Optional	4.2.5
##.DRIFT GAS FLOW=	(AFFN)		Optional	4.2.6
##.CARRIER GAS MOISTURE=	(AFFN)		Optional	4.2.7
##.IONIZATION SOURCE=	(TEXT)		Optional	4.2.8
##.SHUTTER GRID POTENTIAL=	(AFFN)		Optional	4.2.9
##.REPETITION RATE=	(AFFN)		Optional	4.2.10
##.AVERAGES=	(AFFN)		Optional	4.2.11

EXAMPLE JCAMP-DX-FILE FOR IMS DATA EXCHANGE
    ##TITLE=EXAMPLE JCAMP-DX FILE FOR IMS
    ##JCAMP-DX=5.01 $$ ISAS JCAMP-DX program for IMS (V.1.0)
    ##DATA TYPE=ION MOBILITY SPECTRUM
    ##DATA CLASS=XYDATA
    ##ORIGIN=J.I. Baumbach, H. Schmidt, ISAS Dortmund, Germany

##OWNER=COPYRIGHT (C) 2000 by ISAS Dortmund, Germany
##LONG DATE=2000/09/28 14:24:38 +0100
##SOURCE REFERENCE=P:\Hartwig\Messung\000928\H1092801
##NAMES=Tetrachloroethene
##CAS REGISTRY NO=127-18-4
##CONCENTRATIONS=(NCU)
(TETRACHLOROETHENE, 0.46, ppm)
##SPECTROMETER/DATA SYSTEM=ISAS/TE/TE-lang
##.IMS PRESSURE=101
##.CARRIER GAS=NITROGEN
##.DRIFT GAS=NITROGEN
##.ELECTRIC FIELD=-158,-294
##.ION POLARITY=NEGATIVE
##.IONIZATION MODE=PD
##.IMS TEMPERATURE=25.0
##.SHUTTER OPENING TIME=300 $$ microseconds
##.REDUCED MOBILITY=(KA)
(2.38, <tetrachloroethene>)
(2.27, <tetrachloroethene>)
(2.06, <tetrachloroethene>)
(1.83, <tetrachloroethene>)
##.IONIZATION CHAMBER=CYL,30,7.5
##.DRIFT CHAMBER=CYL,120,7.5
##.CARRIER GAS FLOW=0.2
##.DRIFT GAS FLOW=0.11
##.CARRIER GAS MOISTURE=0.03
##.IONIZATION SOURCE= Partial Discharge, Needle= Stainless Steel, Gap = 4.6 mm
##.SHUTTER GRID POTENTIAL=100
##.REPETITION RATE= 100 $$ milliseconds
##XLABEL=Drift Time / ms
##YLABEL=Ion Current / pA
##XUNITS=MILLISECONDS
##YUNITS=PICOAMPERES
##XFACTOR=0.1830348E-02
##YFACTOR=0.1037643E-01
##FIRSTX=0
##LASTX=59.975
##NPOINTS=2400
##FIRSTY=0. 4491087E+01
##XYDATA=(X++(Y..Y))
0D33k31J0844J6532N189j595k202m79K87J50R4r4k02m3J42m808j8005q458M14K093Q14
273H75l8j74q4j41m8K64r9j27J22p5l3M3%J27m3j03J9k4N6R5m3j13%Q5O6r4j18N2J4%
683D61J41q5m7o1Q5K3J0q5Q5j27n2J93l8J04j22r0M3P9j8Q0j13N6P5j17N2l3Rk3j23J79
...
32426C53L7K45m2r0j17M2J04q5J41l3j93J46rJ8K4o6K8J0j41Q9o1J13n2j4O6
32767E13
##END=

6. REFERENCES

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