Exchange, interpretation, and database-search
of ion mobility spectra supported by data format JCAMP-DX

J.I. Baumbach, A.N. Davies, A.v. Irmer, P.H. Lampen

Institut für Spektrochemie und angewandte Spektroskopie,

Bunsen-Kirchhoff-Str. 11, D-44139 Dortmund, Germany

ABSTRACT

To assist peak assignment in ion mobility spectrometry it is important to have quality reference data. The reference collection should be stored in a database system which is capable of being searched using spectral or substance information. We propose to build such a database customized for ion mobility spectra. To start off with it is important to quickly reach a critical mass of data in the collection. We wish to obtain as many spectra combined with their IMS parameters as possible. Spectra suppliers will be rewarded for their participation with access to the database. 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 spectra. The format should be computer readable and flexible enough for extensive comments to be included. In this document we propose a data exchange format, and we would like you to give comments on it.

For the international data exchange it is important, to have a standard data exchange format. We propose to base the definition of this format on the JCAMP-DX protocol, which was developed for the exchange of infrared spectra. This standard made by the **J**oint **C**ommittee on **A**tomic and **M**olecular **P**hysical Data is of a flexible design. The aim of this paper is to adopt JCAMP-DX to the special requirements of ion mobility spectra.
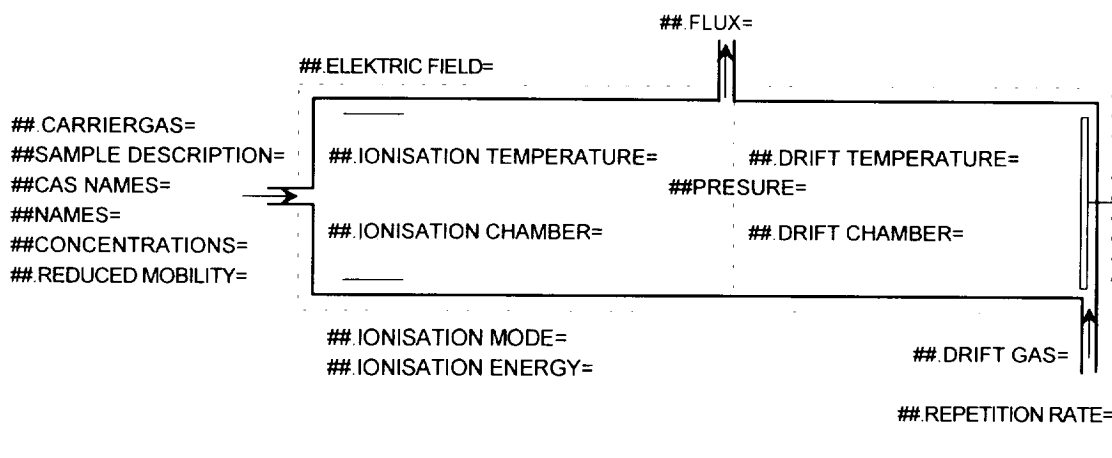
KEY WORDS

Data exchange, ion mobility spectrometry, JCAMP-DX

1   INTRODUCTION

JCAMP-DX is a file based format using ASCII characters (American Standard Code of Information Interchanging) reduced to the printable character. This guarantees the acceptance on all computer systems. The main components to describe the ion mobility spectrometer and the spectra are shown in Figure 1:

Figure 1:

##.FLUX=

##.ELEKTRIC FIELD=

##.CARRIERGAS=
##SAMPLE DESCRIPTION=
##CAS NAMES=
##NAMES=
##CONCENTRATIONS=
##.REDUCED MOBILITY=

##.IONISATION TEMPERATURE=   ##.DRIFT TEMPERATURE=
                                    ##PRESURE=
##.IONISATION CHAMBER=   ##.DRIFT CHAMBER=

##.IONISATION MODE=
##.IONISATION ENERGY=   ##.DRIFT GAS=

                                    ##.REPETITION RATE=

Main declarations to connect ion mobility spectrometry and JCAMP-DX

2   DEFINITIONS

The following definitions are important for the unterstanding of the JCAMP-DX protocol:

2.1   LDR

Labeled-Data-Records (LDR) consists of 80 characters (or less) starting with Data-Labels delimited by ## and terminated with =. For example ##TITLE= is a data lable for the definition of the working title of the following spectrum. There are two kinds of LDR: Core and Note. Core LDRs are required. Notes are optional. Every defintion of an LDR should include if it´s a core or a note.

2.2   TEXT

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

2.3 STRING

Some LDR contain pre-defined text fields intended to be parsed by computers and read by human. The form 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 witch the field must be multiplied. It is followed by + or - and up to three digits. The numeric field is terminated either by E, comma or blank.

2.5 ASDF

This is the ASCII sqeezed difference form. Tabular data using JCAMP-DX data compression scheme. (see section 3.2.9)

3 JCAMP-DX LABELED-DATA-RECORDS (LDR)

The main structure of a JCAMP-DX file consist of

- equipment parameter
- header which includes all file informations
- parameter of spectrum
- sample parameters

3.1 Equipment Parameter

Many LDR are already defined by JCAMP-DX. They can be easy adapted for IM-Spectrometer. But in the case of the equipment parameters the special requirements of this technology call for some special LDRs. The JCAMP-DX standard is easy to expand. Any new LDR starts with "##.". In the following part a conglomerate of definitions coming from IR-, NMR-, MS-JCAMP and special for IMS defined LDR will allow a precise description of the equipment parameters.

3.1.1 ##DATA SYSTEM= (TEXT)

This LDR allows a description of the data acquisition and the treatment of the data. *(Note)*

3.1.2   ##DATA PROCESSING= (TEXT)

Here all mathematical procedures used before storing the data in JCAMP-DX file are described. Even for a peak assignment table this LDR is important. *(Note)*

3.1.3   ##PRESSURE= (STRING)

Pressure inside the IMS-System is ment (in SI-units). *(Note in JCAMP-DX but in this case strongly recommended)*

3.1.4   ##.CARRIERGAS= (TEXT)

A description of the carrier gas is required here. *(Core)*

3.1.5   ##.REDUCED MOBILITY= (AFFN)

In addition of the sample description seen above in this LDR the known reduced mobility can be given. *(Note)*

3.1.6   ##.ELECTRIC FIELD= (AFFN,AFFN)

The electric field description is divided in two parts: The filed in the ionisation chamber and the one in the drift chamber (in Volt / cm). *(Core)*

3.1.7   ##.IONISATION MODE= (STRING)

How does the system ionise the gas? The following keywords are defined:

UV   ultraviolet source

BR   beta-radiation source

For detailed information it is possible to give a comment like $$Ni63-source. *(Core)*

3.1.8   ##.IONISATION ENERGY= (AFFN)

To have the information, witch part of the probe is ionised the ionisation energy is needful (eV is used). *(Note)*

3.1.9   ##.IONISATION TEMPERATURE= (STRING) and ##.DRIFT
         TEMPERATURE= (STRING)

Here the temperature in the ionisation/drift chamber is meant (in °C). *(Core)*

3.1.10   ##TEMPERATURE= (STRING)

The sample temperature in °C should only be given if there is a significant different to room temperature. *(Core)*

3.1.11   ##.IONISATION CHAMBER= (STRING, AFFN, AFFN[, AFFN]) and
         ##.DRIFT CHAMBER= (STRING, AFFN, AFFN[, AFFN])

Different geometrical parameters of the ionisation/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.

(Note)

3.1.12   ##.FLUX= (AFFN, AFFN)

This LDR is divided in two fluxes. The first value is linked to the ionisation chamber and the second to the drift chamber. All values have the unit liter/minute. *(Note)*

After having discussed the IMS equipment LDR´s we now come to the LDR´s which already defined in JCAMP-DX. The header of a file, the spectrum parameter and the sample parameter are nearly the same for other analytical processes. This allows us to adapt most of the standart LDR from the existing JCAMP-DX with some small changes only. For more information see [1], [2] and [3].

3.2   Header

3.2.1   ##TITLE= (TEXT)

Title and/or reason of the measurement. *(Core)*

3.2.2   ##JCAMP-DX= (STRING)

The version number of the used format is 5.00 *(Core)*

3.2.3   ##DATA TYPE= (STRING)

Keywords: ION MOBILITY SPECTRUM or

                             IMS PEAK TABLE

Give a possibility to distinguish between different kinds of data like NMR- or IR-data. The

string ION MOBILITY SPECTRUM reports a continuous spectrum located at the

##XYDATA=-LDR and IMS PEAK TABLE reports distinct and analysed peak's located in

the ##PEAK TABLE=-LDR. *(Core)*

3.2.4   ##DATA CLASS= (STRING)

Keywords: XYDATA or

                             PEAK TABLE

This lable defines the type of tabular data within the data block and is not to be used for link

blocks. *(Core)*

3.2.5   ##ORIGIN= (TEXT)

Here the name of organisation, address, telephone number, name of individual contributor

etc. must be added. This information is <u>not</u> optional.*(Core)*

3.2.6   ##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 the one is named under

##ORIGIN=.*(Core)*

3.2.7   ##DATE= (STRING)

Date of measurement is required here in the form: YY/MM/DD. *(NOTE)*

3.2.8   ##TIME= (STRING)

Time of measurement in the form: HH:MM:SS. *(NOTE)*

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

These records are to be used in compound JCAMP-DX files to provide inter-block refering. A unique positve 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 to use separate files for each data block. *(Core only for compound files)*

EXAMPLE:

##TITLE=	'title of the whole compound file'
##JCAMP-DX=	5.00 $$name & Version No. of JCAMP-DX software
##DATA TYPE=	LINK
##BLOCKS=	'n'
##ORIGIN=	'name of contributor, organisation,
	address, telephone etc.'
##OWNER=	COPYRIGHT (C) 'year' by 'name'
	$$ or PUBLIC DOMAIN
##TITLE=	'title of the first data block'
##JCAMP-DX=	5.00
##DATA TYPE=	ION MOBILITY SPECTRUM
##DATA CLASS=	XYDATA
##BLOCK_ID=	1
##ORIGIN=	'name of contributor, organisation,
	address, telephone etc.'
##OWNER=	COPYRIGHT (C) 'year' by 'name'
	$$ or PUBLIC DOMAIN
##CROSS REFEERENCE=	IMS PEAK TABLE:BLOCK_ID=2
. . .	
##END=	
##TITLE=	'title of the second data block'
##JCAMP-DX=	5.00
##DATA TYPE=	IMS PEAK TABLE
##DATA CLASS=	PEAK TABLE
##BLOCK_ID=	2

```
##ORIGIN=              'name of contributor, organisation,
                       address, telephone etc.'
##OWNER=               COPYRIGHT (C) 'year' by 'name'
                       $$ or PUBLIC DOMAIN
##CROSS REFEERENCE=    ION MOBILITY SPECTRUM: BLOCK_ID=1
   .  .  .
##END=
```

3.2.10   ##SOURCE REFERENCE= (TEXT)

Here an identification to locate the original spectrum file or library name and serial number is possible. *(Note)*

3.2.11   ##CROSS REFERENCE= (TEXT)

If there's additional data for the same sample like peak assignments or other types of spectra, this LDR gives the linkage to them. *(Note)*

EXAMPLE:

```
##CROSS REFERNCE= ION MOBILITY SPECTRUM:
                       EXTERNAL_FILE= FILENAME.DX
                       IMS PEAK TABLE: BLOCK_ID=16
```

3.2.12   ##END=

It's important to have a mark at the end of file in the data format to know that it is complete received and to distinguish between the blocks of a multi spectrum file. *(Core)*

3.3   Parameters of the spectrum

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

Here the units of the axis can be given. The following keywords are defined:
SECONDS, MILLISECONDS, NANOSECONDS, MILLIAMPERS, NANOAMPERS.
(Core)

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

First and last actual abscissa values of ##XYDATA=. First tabulated abbscissa times ##XFACTOR= should equal ##FIRSTX=. *(Core for spectrum files)*

3.3.3   ##FIRSTY= (AFFN)

Here the actual Y-value corresponding to ##FIRSTX= is ment. ##FIRSTY= should be equal ##YFACTOR= times the first Y-value in ##XYDATA=. *(Core for spectrum files)*

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

The values of spectrum have to be integer to save space and allow the DIFDUP format (see 3.2.6). For that the ##XFACTOR=- and ##YFACTOR=-LDR contain a floatingpoint number to be multiplied by the ##XYDATA= values. For example if ##XFACTOR= 0.0001 the following ##XYDATA= 9999 means an X-value of 0.9999. *(Core for spectrum files)*

3.3.5   ##NPOINTS= (AFFN)

Here the numbers of points are required for both cases: IMS-Peak table and IM-Spectrum. *(Core)*

3.3.6   ##XYDATA= (STRING)

This LDR contains spectral data. It is followed by the form of the tabular data like: (X++(Y..Y)) where .. indicate indefinite repeat of Y-values until the end of line and ++ indicates that X is incremented by (##LASTX=-##FIRSTX=)/(##NPOINTS=-1) between two Y. For discrete point the indication (XY..XY) is useable. (See the following example)

This format creates on one hand large files, but is one the other hand readable.
To have a better data compression it is possible to use the squeezed form (SQZ) in witch the delimiter, the leading digit and sign are replaced by a pseudo-digit from Table I.
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 I. To check data, each line starts with the absolute x- and y-value,

witch is the same as the last calculated value of the previous line. The last line of a block of DIF data contains only abscissa and ordinate for y-value check of the last ordinate.

Another possible format is duplicate suppression (DUP) replaces two or more adjacent and identical numbers with pseudo-digits written in Table I. For example 50 50 50 50 becomes 50V. The two formats DIF and DUP can be combined to the most compressing but less readable format called DIFDUP. In this format the duplicate count is obtained by counting identical differences. The example above becomes 50 % % % in DIF form and 50%U in DIFDUP form. *(Core for spectrum files)*

Table I:

Pseudo digits used to compress spectra data in SQS-, DIF- and DUP-format										
ASCII digits	0	1	2	3	4	5	6	7	8	9
Postive 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

Example for normal data storage

Normal form:

```
##YUNITS= NANOAMPER
##XUNITS= MILLISECONDS
##XFACTOR= 1
##YFACTOR= 0.1
##XYDATA= (X++(Y..Y)
4          0   0   0   0   2   4   4   4   7
12         5   4   4   5   5   7  10  11  11
21         6   5   7   6   9   9   7  10  10
31         9  10  11  12  15  16  16  14  17
39        38  38  35  38  42  47  54  59  66
48        75  78  88  96 104 110 121 128
```

103

witch is the same as the last calculated value of the previous line. The last line of a block of DIF data contains only abscissa and ordinate for y-value check of the last ordinate.

Another possible format is duplicate suppression (DUP) replaces two or more adjacent and identical numbers with pseudo-digits written in Table I. For example 50 50 50 50 becomes 50V. The two formats DIF and DUP can be combined to the most compressing but less readable format called DIFDUP. In this format the duplicate count is obtained by counting identical differences. The example above becomes 50 % % % in DIF form and 50%U in DIFDUP form. *(Core for spectrum files)*

Table I:

Pseudo digits used to compress spectra data in SQS-, DIF- and DUP-format

ASCII digits	0	1	2	3	4	5	6	7	8	9
Postive 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

Example for normal data storage

Normal form:

```
##YUNITS= NANOAMPER
##XUNITS= MILLISECONDS
##XFACTOR= 1
##YFACTOR= 0.1
##XYDATA= (X++(Y..Y)
4          0   0   0   0   2   4   4   4   7
12         5   4   4   5   5   7  10  11  11
21         6   5   7   6   9   9   7  10  10
31         9  10  11  12  15  16  16  14  17
39        38  38  35  38  42  47  54  59  66
48        75  78  88  96 104 110 121 128
```

Example for DIFDUP-form

```
##YUNITS= NANOAMPER
##XUNITS= MILLISECONDS
##XFACTOR= 1
##YFACTOR= 0.1
##XYDATA= (X++(Y..Y)
4@VKT%TLkj%J%KLJ%njKjL%kL%jJULJ%kLK1%1LMNPNPRLJ0QTOJ1P
56A28
```

3.3.7 ##PEAK ASSIGNMENT= (STRING)

Keywords: (XA),(XYA) or (XYWA)

After this LDR a list of peak's 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 indicates the location and height of each peak in units given by ##YUNITS= and ##XUNITS=. W stands for width and A represents a string describing the assignment enclosed in angle brackets.

The parentheses are just to get a beginning and ending flag of each assignment. Square backets 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 ASSIGNMENT= -LDR with (XA),(XYA) or (XYWA). This LDR should be followed by a comment, which gives the method of finding the peak. *(Core for peak assignments)*

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

These LDRs give the possibility of labelling the axis. *(Note)*

3.4 Sample information

At least one of the optional LDRs described in this section should be included in each JCAMP-DX file.

3.4.1 ##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. *(Note)*

3.4.2 ##CAS NAME= (STRING)

Name according to Chemical Abstracts naming conventions as described in Appendix IV of the 1985 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-/Superscribts are indicated by prefixes / and ∧. Example: alpha-D-glucopyranose, 1-(dihydrogen phosphate).*(Note)*

3.4.3 ##NAMES= (STRING)

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

3.4.4 ##MOLFORM= (STRING)

Another possibility of describing the sample is to write down the Molecular formular. 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 capitalised. The second letter, if required, is lower case. One-letter symbols must be separated from the next symbol by a blank or digit. Sub-/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. *(Note)*
Examples:

C2H4O2 or C2 H4 O2   (acetic acid)

C6 H9 Cr O6 * H2 O   (chromic acetate monohydrate)

H2 ∧ 17O   (water, mass 17 oxygen)

3.4.5 ##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.

(Note in JCAMP-DX but in this case strongly recommended)

```
##CONCENTRATIONS=  (NCU)
(N₂ ,C₁ ,U₁)

  .  .  .

(N₁ ,C₁ ,U₁)
```

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

4 SUMMERY

In the following tables all discussed LDR's are shown with their basic Parameters:

Equipment Parameter:

LDR	Parameter	Keyword	Status	Location
##DATA SYSTEM=	(TEXT)		Note	3.1.1
##DATA PROCESSING=	(TEXT)		Note	3.1.2
##PRESSURE=	(STRING)		Note in JCAMP-DX but in this case strogly recommended	3.1.3
##.CARRIERGAS=	(TEXT)		Core	3.1.4
##.REDUCED MOBILITY=	(AFFN)		Note	3.1.5
##.ELECTRIC FIELD=	(AFFN, AFFN)		Core	3.1.6
##.IONISATION MODE=	(STRING)	UV or BR	Core	3.1.7
##.IONISATION ENERGY=	(AFFN)		Note	3.1.8
##.IONISATION TEMPERATURE=	(STRING)		Core	3.1.9
##.DRIFT TEMPERATURE=	(STRING)		Core	3.1.9
##TEMPERATUR=	(STRING)		Core	3.1.10
##.IONISATION CHAMBER=	(STRING, AFFN, AFFN [, AFFN])	RECT or CYL	Note	3.1.11
##.DRIFT CHAMBER=	(STRING, AFFN, AFFN [, AFFN])	RECT or CYL	Note	3.1.11
##.FLUX= (AFFN, AFFN)	(AFFN, AFFN)		Note	3.1.12

Header

LDR	Parameter	Keyword	Status	Location
##TITLE=	(TEXT)		Core	3.2.1
##JCAMP-DX=	(STRING)	5	Core	3.2.2
##DATA TYPE=	(STRING)	ION MOBILITY SPECTRUM or IMS PEAKTABLE	Core	3.2.3
##DATA CLASS=	(STRING)	XYDATA or PEAK TABLE	Core	3.2.4
##ORIGIN=	(TEXT)		Core	3.2.5
##OWNER=	(TEXT)		Core	3.2.6
##DATE=	(STRING)		Core	3.2.7
##TIME=	(STRING)		Note	3.2.8
##BLOCK_ID=	(AFFN)		Core for compound files	3.2.9
##BLOCKS=	(AFFN)		Core for compound files	3.2.9
##SOURCE REFERENCE=	(TEXT)		Note	3.2.10
##CROSS REFERENCE=	(TEXT)		Note	3.2.11
##END=			Core	3.2.12

Parameter of Spectrum

LDR	Parameter	Keyword	Status	Location
##XUNITS=	(STRING)	SECONDS, MILLISEC-ONDS, NANOSECONDS	Core	3.3.1
##YUNITS=	(STRING)	MIL-LIAMPERS, NANOAMPERS	Core	3.3.1
##FIRSTX=	(AFFN)		Core for spectrum files	3.3.3
##LASTX=	(AFFN)		Core for spectrum files	3.3.4
##FIRSTY=	(AFFN)		Core for spectrum files	3.3.5
##XFACTOR=	(AFFN)		Core for spectrum files	3.3.6
##YFACTOR=	(AFFN)		Core for spectrum files	3.3.7
##NPOINTS=	(AFFN)		Core for spectrum files	3.3.8
##XYDATA=	(STRING)	(X++(Y..Y)), (XY..XY)	Core for spectrum files	3.3.9
##PEAK ASSIGNMENT=	(STRING)	(XA),(XYA) or (XYWA)	Core for peak assignments	3.3.10
##XLABLE=	(TEXT)		Note	3.3.11
##YLABLE=	(TEXT)		Note	3.3.12

Header

LDR	Parameter	Keyword	Status	Location
##TITLE=	(TEXT)		Core	3.2.1
##JCAMP-DX=	(STRING)	5	Core	3.2.2
##DATA TYPE=	(STRING)	ION MOBILITY SPECTRUM or IMS PEAKTABLE	Core	3.2.3
##DATA CLASS=	(STRING)	XYDATA or PEAK TABLE	Core	3.2.4
##ORIGIN=	(TEXT)		Core	3.2.5
##OWNER=	(TEXT)		Core	3.2.6
##DATE=	(STRING)		Core	3.2.7
##TIME=	(STRING)		Note	3.2.8
##BLOCK_ID=	(AFFN)		Core for compound files	3.2.9
##BLOCKS=	(AFFN)		Core for compound files	3.2.9
##SOURCE REFERENCE=	(TEXT)		Note	3.2.10
##CROSS REFERENCE=	(TEXT)		Note	3.2.11
##END=			Core	3.2.12

Parameter of Spectrum

LDR	Parameter	Keyword	Status	Location
##XUNITS=	(STRING)	SECONDS, MILLISEC-ONDS, NANOSECONDS	Core	3.3.1
##YUNITS=	(STRING)	MIL-LIAMPERS, NANOAMPERS	Core	3.3.1
##FIRSTX=	(AFFN)		Core for spectrum files	3.3.3
##LASTX=	(AFFN)		Core for spectrum files	3.3.4
##FIRSTY=	(AFFN)		Core for spectrum files	3.3.5
##XFACTOR=	(AFFN)		Core for spectrum files	3.3.6
##YFACTOR=	(AFFN)		Core for spectrum files	3.3.7
##NPOINTS=	(AFFN)		Core for spectrum files	3.3.8
##XYDATA=	(STRING)	(X++(Y..Y)), (XY..XY)	Core for spectrum files	3.3.9
##PEAK ASSIGNMENT=	(STRING)	(XA),(XYA) or (XYWA)	Core for peak assignments	3.3.10
##XLABLE=	(TEXT)		Note	3.3.11
##YLABLE=	(TEXT)		Note	3.3.12

```
13  512,4864,4608,4096,4096,4096,4096,4096,4096,4352
14  4352,4608,4608,4864,4864,4608,4608,512,512,4864
15  4864,4608,4608,4608,512,512,4864,4608,4608,4864
16  5376,4864,4352,4096,4352,4608,4864,512,4864,512
17  512,5376,5376,512,4608,4608,4608,4864,4864,512
18  512,4864,4864,512,5376,5376,512,512,512,512
19  5376,5376,5888,6144,6912,8448,107520,135680,168960,20480
20  225280,245760,245760,23040,207360,176640,151040,133120,122880,107520
21  104960,107520,122880,133120,156160,174080,184320,186880,181760,174080
22  163840,14080,122880,107520,9472,896,896,896,8704,8704
23  9216,104960,122880,130560,14080,145920,143360,138240,1280,112640
24  9472,8192,6912,6656,64,6656,64,6144,5888,5888
25  512
##XLABLE=Drifttime /ms
##YLABLE=Ion Current /A
##END=
```

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