IUPAC / JCAMP-DX: An International Standard for the Exchange of Ion Mobility Spectrometry Data

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ABSTRACT

For safe international data exchange it is important, to have an agreed manufacturer independent standard data exchange format. A standard is proposed for ion mobility spectrometry based on the JCAMP-DX protocol.
This standard protocol was initially developed for the exchange of infrared spectra (1988) and has been followed by equivalent standards for Chemical Structure (1991), Nuclear Magnetic Resonance spectroscopy (1993) and Mass Spectrometry (1994) [1-4].

In order to produce a standard for use by the Ion Mobility Spectrometry community a *DATA DICTIONARY* needs to be agreed upon containing the keywords particular to IMS. This list of keywords is presented and a request is made for detailed discussion and suggestions for addition and subtraction from the list.

The IMS User Community must agree on the keywords required for this technique by July 1998 then the paper will be presented through the IUPAC Working Party on Spectroscopic Data Standards (JCAMP-DX) to the Committee on Printed and Electronic Publications for acceptance as a IUPAC standard.

INTRODUCTION

In order to decide on the content of the Data Dictionary all workers in the field of Ion Mobility Spectrometry (IMS) should examine their experimental arrangements such as that shown in figure 1 and decide whether or not they can use the IMS specific data fields listed in Table 1 to completely describe their experiment. Subsidiary information is always stored using labels which are not spectroscopy-type specific and references 1-4 should be referred to for these labels.

The following definitions are important to understand the JCAMP-DX protocol and Table 1:

- LDR
  Labeled-Data-Records (LDR) consists of 80 characters (or less) on one line, unlimited number of lines, starting with Data-Labels delimited by ## and terminated with =. For example ##TITLE= is a data label for the definition of the working title of the spectrum. There are two kinds of LDR: Core and Note. Core LDRs are required. Notes are optional.

- TEXT
  Text LDRs contain descriptive information for humans, with no fixed format.

- STRING
  Some LDRs contain predefined text fields intended to be parsed by computers and read by humans. The allowed form of each string field is specified under the individual LDR definition.

- 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.

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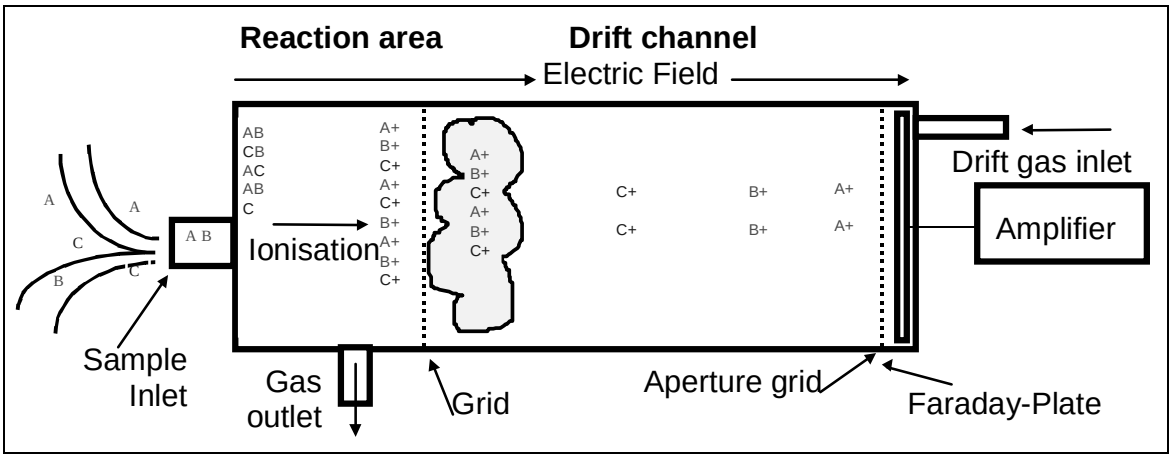

Figure 1: Can you describe your experimental data with the current data dictionary in table 1?

- ASDF
  This is the ASCII squeezed difference form. A data compression scheme unique to JCAMP-DX which dramatically reduces the file size without any loss of information.

If it is possible to describe every aspect of your IMS experiment with the current data dictionary then no changes need to be suggested and if this is the general case then shortly an international independent data exchange standard will be available for Ion Mobility Spectrometry data. A short example file is shown in table 2. If however it is not then we need your input to ensure the IUPAC standard meets ALL the needs of the IMS user community. To this end a committee was set up consisting of David Atkinson (Lockheed Martin Idaho Technologies, Idaho Falls, ID), Gary Eiceman (New Mexico State University, Las Cruces, NM) and the authors to decide on the fields required for the data dictionary.

WWW Information

In order to keep interested parties up-to-date on the latest developments in this field the Internet Web Site of the IUPAC Working Party will always show the status of the data standards under development and make the protocols available when they are complete. For further information see:
http://www.isas-dortmund.de/projects/jcamp

This information will be accessible from this side although the exact web address will alter as the status of the new protocol changes.

Table 1: Draft list of IMS-SPECIFIC LDRs

LDR	Data form	Keyword	Status	Reference
##DATA SYSTEM=	(TEXT)		Note	3.1.1
##DATA PROCESSING=	(TEXT)		Note	3.1.2
##PRESSURE=	(STRING)		Note	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 BETA*	Core	3.1.7
##.IONISATION ENERGY=	(AFFN)		Note	3.1.8
##.IONISATION TEMPERATURE=	AFFN		Core	3.1.9
##.DRIFT TEMPERATURE=	(AFFN		Core	3.1.9
##TEMPERATURE=	(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
##DATA TYPE=	(STRING)	*ION MOBILITY SPECTRUM or IMS PEAKTABLE*	Core	3.2.3
##XUNITS=	(STRING)	*SECONDS or MILLISECONDS or MICROSECONDS or NANOSECONDS*	Core	3.3.1
##YUNITS=	(STRING)	*MILLIAMPERES or MICROAMPERES or NANOAMPERES*	Core	3.3.1

Table 2: EXAMPLE JCAMP-DX-FILE FOR IMS DATA EXCHANGE

```
##TITLE=Example for a JCAMP-DX file for IMS
##JCAMP-DX=5.00
##DATATYPE=ION MOBILITY SPECTRUM
##DATA CLASS=XYDATA
##ORIGIN= A.v.Irmer, ISAS Dortmund, Germany
##OWNER=COPYRIGHT (C) 1997 by ISAS Dortmund, Germany
##DATE=94/09/12
##TIME=12:37:23
##SOURCE REFERENCE=C:\VONIRMER\AVIJIBB.ASC
##Data System=PCI28000
##DATA PROCESSING=AVIJIBBOVERSAMPLING
##PRESSURE=101
##.CARRIERGAS=ARGON
##.ELECTRIC FIELD=(250,333)
##.IONISATION MODE=BR  $$Ni63
##.IONISATION TEMPERATURE=25
##.DRIFT TEMPERATURE=25
##TEMPERATURE=25
##.IONISATION CHAMBER=(CYL,2,2)
##.DRIFT CHAMBER=(CYL,5,2)
##.FLUX=(2,5)
##XUNITS=MILLISECONDS
##YUNITS=AMPERES
##XLABELE= Drift time /ms
##YLABEL= Ion Current /A
##FIRSTX=10
##LASTX=25
##FIRSTY=4.096E11
##XFACTOR=1
##YFACTOR=1E7
##NPOINTS=151
##XYDATA=(X++(Y..Y))
10      4096,4352,4608,4352,4352,4864,4608,4864,4608,4352
11      4096,4096,4352,4352,4096,4096,4096,4352,4512,4608
12      4352,4096,4352,4352,4608,4352,4096,4096,4864,512
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
##END=
```

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