

JCAMP-DX for NMR*

ANTONY N. DAVIES† and PETER LAMPEN

ISAS, Institut für Spektrochemie und angewandte Spektroskopie, Postfach 10 13 52, 44139 Dortmund, Germany

Following the development and publication of the JCAMP-DX protocol 4.24 and its successful implementation in the field of infrared spectroscopy, data exchange without loss of information, between systems of different origin and internal format, has become a reality. The benefits of this system-independent data transfer standard have been recognized by workers in other areas who have expressed a wish for an equivalent, compatible standard in their own fields. This publication details a protocol for the exchange of Nuclear Magnetic Resonance (NMR) spectral data without any loss of information and in a format that is compatible with all storage media and computer systems. The protocol detailed below is designed for spectral data transfer, and its use for NMR imaging data transfer has not as yet been investigated.

Index Headings: Computer applications; NMR.

1. INTRODUCTION

Following discussions in the U.S.A. and Europe it was agreed that the Nuclear Magnetic Resonance (NMR) JCAMP-DX standard would be prepared for implementation under the fledgling Generic JCAMP-DX Version 5.0 format rather than the JCAMP-DX 4.24 compatible form originally envisaged. The commitment of three leading NMR spectrometer manufacturers at the Sixth INUM Conference in Italy 1990 to implement the standard when finished also provided extra impetus to the development. Small changes have been made to the drafts circulated to overcome difficulties observed during initial implementation of the earlier versions. The problems associated with the storage of multidimensional data sets have not yet been fully classified or overcome, so this proposal does not define any special storage format for multi-dimensional NMR experiments outside what is already possible within the Generic JCAMP-DX Version 5.0 "NTUPLE" format. This publication freezes the development of the simple data model for NMR and will be expanded toward multi-dimensional data sets at a later date.

Received 14 January 1993.

* *Contributing Persons:* Antony N. Davies (Coordinator), ISAS Dortmund, F.R.G.; Charles Thibault, Bruker, U.S.A.; Robert S. McDonald, Burnt Hills, U.S.A.; Thomas Kämpchen, University of Marburg, F.R.G.; Heinrich Hillig, ISAS Dortmund, F.R.G.; Reinhard Neudert, BASF, F.R.G.; Dan Iverson, Varian, U.S.A.; Ben Hendriks, Solvay Duphar, The Netherlands; Doug Meinhart JEOL, U.S.A.; Howard Mack, Bran Luebbe, U.S.A.; Peter Lampen and Jörg Lambert, ISAS Dortmund, F.R.G.

† Author to whom correspondence should be sent.

2. SCOPE

This standard was accepted and given free for publication at the JCAMP executive meeting in Chicago on 5 March 1991. The protocol follows the general lines laid down in the JCAMP 4.24¹ protocol and adheres to the design criteria stated therein. It has been expanded to include new features available under Generic JCAMP-DX Version 5.0.^{2,3} The protocol is meant for public use. The specifications are placed in the public domain and right to copy for scientific purposes is hereby granted.

3. FILE STRUCTURES AND DEFINITIONS

File structures and definitions are as defined in sections 3 and 4 of the JCAMP-DX 4.24 protocol.¹ The Generic JCAMP-DX Version 5.0 allows the use of a new NTUPLE data structure. Under JCAMP-DX Version 5.0, the file content is divided into two main sections, the CORE and the NOTES, each section containing the general GLOBAL information common to all JCAMP-DX files and the NMR DATATYPE SPECIFIC information, which is defined in this publication. The datatype-specific labels differ from the global labels in that they are written "`##.labelname=`" rather than "`##labelname=`."

4. DATA REPRESENTATION

Data compression presents a new problem for NMR spectral coding. For NMR spectra, simple data sets contain only real values and can be coded as in infrared spectroscopy, since the imaginary values are not of interest. When an NMR free-induced decay (FID) is to be transferred, there are more factors which are required to enable successful conversion. Phasing and mode of data acquisition should now be included. FIDs will be handled differently depending on whether they originate from a spectrometer with a single detector and analog-to-digital converter (ADC) or with twin detectors and a single ADC. The processing is different again for an FID obtained by normal quad detection.

While we will not go into the benefits of the various methods it is clear that, before an FID from one of these acquisition methods can be converted into the internal storage format of a computer designed to handle data from one of the other methods, a significant amount of

conversion, must take place. To flag the necessary conversion, the datatype-specific LDR `##ACQUISITION MODE=`, with the priority `REQUIRED` for FIDs, will be used.

(4.1) **TABULAR DATA.** If a simple NMR spectrum is to be coded and transferred, then the `##XYDATA=(X++(Y..Y))` format suffices. However, for more effective use of the DIFDUP principle (see Ref. 1, Section 5.10) the real and imaginary data sets of the FID or spectrum should be coded independently. This separate coding requires the use of two independent, cross-referenced blocks or the NTUPLE format.

(4.1.1) **VARIABLE LIST.** The forms of tabular data represented in JCAMP-DX 4.24 continue to be valid here, but in addition several others are presented. To differentiate between real and imaginary data lists, the formats `(X++(R..R))` for real values and `(X++(I..I))` for imaginary values are adopted where `..` continues to indicate indefinite repeat until the line is filled and `++` indicates that X is incremented by `(LASTX-FIRSTX)/(NPOINTS-1)`. Other minor changes are detailed in the text where relevant.

(4.2) **DATA COMPRESSION.** The `AFFN`, `PACKED`, `SQUEEZED`, and `DIFFERENCE` formats are allowed as defined in the JCAMP-DX 4.24 publication (5.2-5.6).¹ The `DIFFERENCE` format is recommended to minimize file storage requirements.

(4.3) **X-SEQUENCE AND Y-VALUE CHECKING.** X-sequence and Y-value checking is to be carried out as specified in JCAMP-DX Version 4.24 (5.8).

(4.4) **DUPLICATE SUPPRESSION.** Duplicate suppression can be carried out as detailed in the JCAMP-DX 4.24 protocol (5.9).

5. THE CORE

This section describes the data labels for the JCAMP-DX NMR core data. The Core consists of four parts. The first part, called the "Fixed Header Information," contains generic label data records (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 which are datatype specific (in this case NMR-specific) or which are used only in special types of JCAMP-DX files (e.g., compound files). Whether a particular LDR is required or not depends on the application. The third section, "Core Data," contains the spectral parameters for the fourth section, the "Data Table." The type of data in the data table determines the parameters which 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=`).

(5.1) CORE FIXED HEADER INFORMATION.

(5.1.1) `##TITLE=`, and `##JCAMP-DX=`, are defined as in the DX 4.24 protocol (6.1)¹ and have the priority `REQUIRED`. `##JCAMP-DX=` has the value 5.00. The `##JCAMP-DX=5.00` LDR should be followed by a `$$` comment on the same line identifying the software producing the data file.

(5.1.2) `##DATA TYPE= (STRING)` is expanded to

include the values `NMR FID`, `NMR SPECTRUM`, `NMR PEAK TABLE`, or `NMR PEAK ASSIGNMENTS` and has the priority `REQUIRED`.

(5.1.3) `##DATA CLASS= (STRING)` contains `XY-DATA`, `XYPOINTS`, `PEAK TABLE`, `ASSIGNMENTS`, or `NTUPLES`. The label is priority `WARN` and should be included. This label defines the type of tabular data within the data block and is not to be used for link blocks.

(5.1.4) Two labels, `##ORIGIN=` and `##OWNER=`, have the priority `WARN` and should be included. Software developers should ensure that a JCAMP-DX file cannot be created with these fields left blank.

(5.2) CORE VARIABLE HEADER INFORMATION.

(5.2.1) `##BLOCKS=`, and `##BLOCK_ID= (STRING)` 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)⁴ to provide inter-block referencing. When, for example, `XYDATA` and a `PEAK TABLE` are to be stored, these must be written as a compound file¹ (see also section 5.4 below). 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 unique positive integer should be given to each block inside the compound JCAMP-DX file. Linking of the blocks can then be achieved with the use of `##CROSS REFERENCE=` (see example 4).

(5.2.2) `##OBSERVE FREQUENCY= (AFFN)`. Observer frequency in MHz. Priority `REQUIRED`.

(5.2.3) `##OBSERVE NUCLEUS= (STRING)`. Observed nucleus written as described in JCAMP-DX 4.24 section (7.2.4)¹ (i.e., `^13C`). This LDR has the priority `REQUIRED`.

(5.2.4) `##SOLVENT REFERENCE= (AFFN)`. Solvent lock signal in ppm. Priority `REQUIRED` if a solvent lock signal was used instead of TMS.

(5.2.5) `##DELAY= (RD, ID)`. Pre-acquisition delays for the real values (RD) and the imaginary values (ID) in μ s. This agreement allows for the storage of simultaneously recorded real and imaginary data FIDs where the two delays will be identical, or alternating recorded real and imaginary FIDs where the two delays will be different. This LDR has the priority `REQUIRED` in `##DATATYPE= NMR FID` but priority `OPTIONAL` for `##DATATYPE= NMR SPECTRUM`, `NMR PEAK TABLE`, and `NMR PEAK ASSIGNMENTS`.

(5.2.6) `##ACQUISITION MODE= (STRING)`. This LDR has the priority `REQUIRED` for `##DATATYPE= NMR FID` but only `OPTIONAL` for `NMR SPECTRUM`, `NMR PEAK TABLE`, and `NMR PEAK ASSIGNMENTS`. It can take the value `SIMULTANEOUS` for data obtained from true quadrature detection using two detectors and two ADCs, `SINGLE` for Time Proportional Phase Increment detection with a single detector and ADC, and the value `SEQUENTIAL` when data are obtained from two detectors with the use of only a single ADC.

(5.3) CORE DATA.

(5.3.1) `##XUNITS= (STRING)`. For NMR data the following abscissa units can be specified: `SECONDS` for FIDs and `HZ` for spectra. Priority `REQUIRED`. `Hz` and `PPM` are allowed for `PEAK TABLES` and `PEAK ASSIGNMENTS`.

(5.3.2) **##YUNITS= (STRING)**. Should be ARBITRARY UNITS. Priority REQUIRED.

(5.3.3) **##FIRSTX=, ##LASTX= (AFFN)**. Are as defined in the JCAMP-DX 4.24 protocol (6.2.3)¹ with priority REQUIRED for XYDATA.

(5.3.4) **##MAXX=, ##MINX=, ##MAXY=, ##MINY= (AFFN)**. Specifications are as defined in the JCAMP-DX 4.24 protocol (6.2.4)¹ with priority OPTIONAL.

(5.3.5) **##XFACTOR=, ##YFACTOR= (AFFN)**. These labels remain as previously defined in the JCAMP-DX 4.24 protocol (6.2.5)¹ and have the priority REQUIRED for XYDATA.

(5.3.6) **##NPOINTS= (AFFN)**. Gives the number of components of **##XYDATA=, ##XYPOINTS=, ##PEAK TABLE=, or ##PEAK ASSIGNMENTS=** and has the priority REQUIRED. This label is not required for the NTUPLE form where the **##VAR_DIM=** label for the X-variable is sufficient.

(5.3.7) **##FIRSTY= (AFFN)**. Actual Y-value corresponding to **##FIRSTX**. **##FIRSTY=** should equal **##YFACTOR=** times the first Y-value in **##XYDATA=**. Priority WARN for XYDATA.

(5.4) CORE DATA TABLE. This section deals with the different methods of storing the NMR data. The major changes from JCAMP-DX Version 4.24 are the inclusion of the NTUPLE form, which is intended for multiple data sets and will be dealt with separately. *N.B.*: Only one of the following LDRs can be used in each block. To store a spectrum using **##XYDATA=** and also the peaktable using **##PEAK ASSIGNMENTS=**, for example, would require two blocks.

(5.4.1) **##XYDATA= (AFFN or ASDF)**. Contains a table of ordinates at equal intervals specified by parameters defined in section 5.3. The label is followed by a variable list, (X++(Y..Y)), (X++R..R)), or (X++(L..I)). Priority OPTIONAL.

(5.4.1.1) **RECOMMENDED ORDINATE SCALING**. The recommended ordinate scaling between -32768 and 32767 from Version 4.24 remains in force. There are currently few applications in NMR spectroscopy where this dynamic range would be insufficient to code all the relevant information. Gratuitous use of larger ordinate scalings normally provides only accurate transfer of noise! If this range is exceeded, the values of **##MAXY** and **##MINY** must be given.

(5.4.1.2) **ABSCISSA SPACING**. This should be the abscissa of the internal data file. Any manipulation to another form should be carried out by the data system requiring the different internal format. The JCAMP-DX file should remain an exact representation of the original data, allowing conversion back into the original data system without any loss of information.

(5.4.1.3) **ABSCISSA ORDER**. There are no requirements for a particular abscissa ordering, so decoding software must be able to cope with both ascending and descending X-values.

(5.4.1.4) **SPECTRUM SIZE**. There are no restrictions on spectral size. Decoding software must therefore be capable of reducing spectral resolution or extracting relevant spectral regions if the size of the spectrum in the JCAMP-DX file exceeds the internal limits of the receiving system.

(5.4.2) **##XYPOINTS= (AFFN)**. Contains a table of XY pairs and is for use with data which are not at equal abscissa increments. This LDR is followed by a variable list, i.e., (XY..XY), (XR..XR), or (XI..XI). X and Y are separated by commas; pairs are separated by semicolons or blanks. This LDR must not be used for peak tables. Priority OPTIONAL.

(5.4.3) **##PEAK TABLE= (STRING)**. Contains a table of peaks. For abscissa against intensity, the variable list (XY..XY) should be used. For peak position, intensity, and width, the variable list would be (XYW..XYW). The function used to calculate the peak width must be detailed in a \$\$ comment line immediately following the **##PEAK TABLE=** line. For peak position, intensity, and multiplicity, the variable list would be (XYM..XYM) where M stands for multiplicity (being S, D, T, Q for singlets, doublets, triplets, or quadruplets, M for multiple, and U for unassigned). List separators are commas, and group separators are semicolons or new lines.

A weak point in release 4.24 of JCAMP-DX was the inter-block linking. The use of **##BLOCK_ID=** and **##CROSS REFERENCE=** in Version 5.0 now links blocks of different information types. For the following section and (6.2.14) such a link to a JCAMP-CS⁴ structure file is assumed, and the atom numbering of the CS file is carried over into the NMR block.

(5.4.4) **##PEAK ASSIGNMENTS= (STRING)**. List of peak assignments for components or functional groups in the forms **##PEAK ASSIGNMENTS= (XYA), (XYWA), (XYMA), (XYMWA)**. Each entry is surrounded by parentheses and starts a new line. Y, W (peak width), and M (multiplicity) values are optional. The symbol A stands for a string detailing the assignment and must be enclosed by angle brackets. If the peak width value is included, then the function used to calculate the peak width must be detailed in a \$\$ comment on the line(s) below **##PEAK ASSIGNMENTS=**. Priority OPTIONAL. *N.B.*: **##PEAK ASSIGNMENTS=** is the preferred method of transmitting peak information when the assignments are known.

6. THE NOTES

This section describes the data labels used for notes in JCAMP-DX NMR. The inclusion of notes in a JCAMP-DX file provides the opportunity for program designers to include relevant background information pertaining to the spectrum. The choice of labels broadly depends on the application.

(6.1) GLOBAL NOTES. The following parameters are desirable for clarity but must not be used for the conversion of the spectral data. They are used only to provide information during visual inspection of the file.

All sample and miscellaneous information notes detailed in JCAMP-DX Version 4.24 (7.2 and 7.1) are acceptable. Structures should be included in JCAMP-CS format rather than Wiswesser or Beilstein Lawson No. Special note should be made of **##CONCENTRATIONS=**, since this LDR must be used to carry solvent information and the inclusion of any standard in the sample.

The equipment information notes detailed in JCAMP-DX Version 4.24 **##SPECTROMETER/DATA SYS-**

TEM= (STRING), and ##INSTRUMENTAL PARAMETERS= (STRING) are acceptable and are regarded as desirable here. All the sampling information notes designated in 4.24 can be used in NMR except for the label ##PATHLENGTH=.

(6.1.1) ##SAMPLING PROCEDURE= (TEXT). This label can be used for coding the multifarious NMR pulse sequences, pulse delays, pre-acquisition delays, pulse angles, sample spin rates, etc. To define individual keywords would be pointless since the current in-vogue pulse sequences will probably be soon surpassed by others and require that the protocol be updated for every new sequence, which is impractical. Decoupling information can also be included here.

(6.1.2) ##DATA PROCESSING= (TEXT). Information on the data handling should be included here if relevant—line broadening, window functions, filters, etc.—but only when the information is significant to the spectrum. It is normally to be assumed that the spectroscopist making the measurements was competent enough to set day-to-day parameters correctly for his or her instrument and they would therefore not be included in a transfer file.

The various comment formats and the label LDRs from JCAMP-DX Version 4.24 (7.5)¹ are all valid in this protocol. The following spectral parameters are also recommended.

(6.1.3) ##RESOLUTION= (STRING). Nominal resolution for the X-axis. Priority OPTIONAL.

(6.1.4) ##DELTA= (AFFN). Nominal spacing between X-values in Hz for spectra or seconds for FIDs depending on ##XUNITS= often referred to as the sweepwidth. Priority OPTIONAL. The actual spacing must always be calculated with the formula (LASTX - FIRSTX)/(NPOINTS - 1).

(6.2) DATA TYPE SPECIFIC NOTES.

(6.2.1) ##FIELD= (AFFN). The magnetic field strength in Tesla should be included with the use of this label. Priority OPTIONAL.

(6.2.2) ##DECOUPLER= (STRING). Table of decoupler frequencies in the form ##DECOUPLER= (F,90), where frequencies (F) are given in MHz and decoupler 90° pulses (90) in μs. Priority OPTIONAL.

(6.2.3) ##FILTER WIDTH= (AFFN,TEXT). Filter width in Hz followed by a description of the filter algorithm. Priority OPTIONAL.

(6.2.4) ##ACQUISITION TIME= (AFFN). Required for calculations involving resolution. Value given in seconds. Priority OPTIONAL.

(6.2.5) ##ZERO FILL= (AFFN). Number of complex zero filling points used. Priority OPTIONAL.

(6.2.6) ##AVERAGES= (AFFN). Number of transients averaged. Priority OPTIONAL.

(6.2.7) ##DIGITISER RES= (AFFN). Digitizer resolution in bits. Priority OPTIONAL.

(6.2.8) ##SPINNING RATE= (AFFN). Sample spinning rate in Hz. Priority OPTIONAL.

(6.2.9) ##PHASE 0= (AFFN). Zero-order phase correction in degrees. Priority OPTIONAL.

(6.2.10) ##PHASE 1= (AFFN). First-order phase correction in degrees per Hz relative to the maximum X-value. Priority OPTIONAL. If a pivot point other than the maximum X-value was used, then the phase correction figure should be recalculated for a pivot point at maximum X.

(6.2.11) ##MIN INTENSITY= (AFFN). Only for use with peaktables, used to represent the minimum intensity used for peak picking. Priority OPTIONAL.

(6.2.12) ##MAX INTENSITY= (AFFN). Only for use with peaktables, used to represent the maximum intensity used for peak picking. Priority OPTIONAL.

(6.2.13) ##OBSERVE 90= (AFFN). 90 degree observer pulse time in μs. This LDR has the priority OPTIONAL.

(6.2.14) ##COUPLING CONSTANTS= (AFFN). These LDRs appear as a list similar in format to ##PEAK TABLE= but require the JCAMP-CS structure file to also be included and accessible. For heteroatoms ##COUPLING CONSTANTS= should be followed by the variable list J(A,B) where J is the coupling constant in Hz, A the atom number, and B the heteroatom number from the JCAMP-CS connection table. For proton coupling hydrogen B must be explicitly coded in the CS file. Priority OPTIONAL.

(6.2.15) ##RELAXATION TIMES= (AFFN). List of relaxation times with the variable list (XYR) where X and Y are the abscissa and intensity values and R the relaxation time in seconds. Priority OPTIONAL.

7. COMPLEX DATA STORAGE

The new NTUPLE format is designed for multi-dimensional techniques with data sets of more than two variables (by GC-IR, XY and time, for instance). In the NMR JCAMP-DX, the format can be used to solve the problem of the mixed real/imaginary FID data sets. The best method of explaining the new format is with example 1.

Example 1.

```
##TITLE= ETHYLBENZENE/CDCL3
##JCAMP-DX= 5.00 $$ ISAS JCAMP-DX NMR program (draft version)
##DATA TYPE= NMR FID
##DATA CLASS= NTUPLES
##ORIGIN= Dr.J.Lambert, ISAS Dortmund, FRG
##OWNER= Copyright (C) 1992 by ISAS Dortmund, FRG
##OBSERVE FREQUENCY= 100.4
##OBSERVE NUCLEUS= ^13C
##DELAY= (22.5, 22.5)
##ACQUISITION MODE= SIMULTANEOUS
```

```

##SPECTROMETER/DATA SYSTEM= JEOL GX 400
##NTUPLES= NMR FID
##VAR_NAME= TIME, FID/REAL, FID/IMAG, PAGE NUMBER
##SYMBOL= X, R, I, N
##VAR_TYPE= INDEPENDENT, DEPENDENT, DEPENDENT, PAGE
##VAR_FORM= AFFN, ASDF, ASDF, AFFN
##VAR_DIM= 16384, 16384, 16384, 2
##UNITS= SECONDS, ARBITRARY UNITS, ARBITRARY UNITS,
##FIRST= 0.0, 2980, 6216, 1
##LAST= 0.682, -60242, -6064, 2
##MIN= 0.0, -170402, -165286, 1
##MAX= 0.682, 149235, 161918, 2
##FACTOR= 0.4162852E-04, 0.5200415E+01, 0.5044282E+01, 1
##PAGE= N=1
##DATA TABLE= (X++(R..R)), XYDATA $$ Real data points
0E73J0801K743n991j1702J2907o922p342r868p9141924J3049K1127R280J0543p471j2800
...
16376D9680380k283j1121078j2640L506p325
16383a1584 $$ checkpoint
##PAGE= N=2
##DATA TABLE= (X++(I..I)), XYDATA $$ Imaginary data points
0A232J9544101901994j8571p88K0538J355J6653J718N398o027N305L183j909J1943k4401
...
16380h871o791o021Q439
16383a202 $$ checkpoint
##END NTUPLES= NMR FID
##END=

```

Both the real and imaginary data sets can be coded within one block. When the data sets are of variable length, `##NPOINTS=` must follow the `##PAGE=` label, and `##VAR_DIM=` provides the maximum length to be expected. The data-type-specific labels required for FIDs would be placed above this data array section of the file, as with the conventional JCAMP-DX file. The NTUPLE format advantage lies in the simplified data coding offered.

Test files. A disk containing test data files in various formats is available on request from the authors. Further examples of the file formats produced are given in the appendix.

8. CONCLUSIONS

The benefits of the use of standard data transfer formats is no longer in dispute. In a recent publication⁵ the Coblenz Society detailed how JCAMP-DX files should be used in future high-quality infrared spectral collections. They listed the information required to be transmitted with the spectra and the JCAMP-DX keywords under which this information should be stored.

We have recently received and corrected test files from the instrument manufacturers who have been working on implementing the draft version of this document. The problems that arose during these implementations have

been solved, and the necessary adaptations written into the protocol before development was frozen for publication.

A standard which is independent of spectrometer manufacturer and software company will also be of great value to those responsible for installing and maintaining spectroscopic data archives. The danger of not being able to read old electronic data onto new systems will be negated.

ACKNOWLEDGMENTS

The authors would like to thank the German Bundesminister für Forschung und Technologie (BMFT) for financial support and encouragement, and the Ministerium für Wissenschaft und Forschung des Landes Nordrhein-Westfalen, Germany.

1. R. S. McDonald and P. A. Wilks, *Appl. Spectrosc.* **42**, 151 (1988).
2. R. S. McDonald, private communication, "Generic JCAMP-DX Memorandum No. 2" Sept. 4th 1990, Robert S. McDonald, JCAMP-DX subcommittee, 9 Woodside Drive, Burnt Hills, New York 12027, U.S.A.
3. Generic JCAMP-DX, Version 5.0, Draft 1.0 February 28, 1991, R. S. McDonald, JCAMP-DX subcommittee, 9 Woodside Drive, Burnt Hills, New York 12027, U.S.A. (Distributed at PITTCON-91)
4. J. Gasteiger, B. M. P. Hendriks, P. Hoever, C. Jochum, and H. Somberg, *Appl. Spectrosc.* **45**, 4 (1991).
5. K. S. Kalasinsky, P. R. Griffiths, D. F. Gurka, S. R. Lowry, and M. Boruta, *Appl. Spectrosc.* **44**, 211 (1990).

APPENDIX

Example 2: A Test Spectrum.

```
##TITLE= ETHYLBENZENE/CDCL3
##JCAMP-DX= 5.00 $$ ISAS NMR JCAMP-DX program (draft version)
##DATA TYPE= NMR SPECTRUM
##DATA CLASS= XYDATA
##ORIGIN= Dr.J.Lambert, ISAS Dortmund, FRG
##OWNER= Copyright (C) 1992 by ISAS Dortmund, FRG
##.OBSERVE FREQUENCY= 100.4000
##.OBSERVE NUCLEUS= ^13C
##SPECTROMETER/DATA SYSTEM= JEOL GX 400
##RESOLUTION= 1.470000
##DELTA= -1.467283
##XUNITS= HZ
##YUNITS= ARBITRARY UNITS
##XFACTOR= 1.467283
##YFACTOR= 29670.15003
##FIRSTX= 24038.50
##LASTX= 0.000000E+00
##MAXY= 972201806
##MINY= -27593240
##NPOINTS= 16384
##FIRSTY= 2254931
##XYDATA= (X++(Y..Y))
16383G6k53o5J88M13k12k70J95K00k1301q3k25J80k9j20MQ6j16n7J70J57NL8q9N1M0k95
16356a63J98K3J59m73m8J80J10M1k28k55J83J45r2K59R5k82p8j9L50j12QM7j82K30117
...
59b10P0J9r2j02K9N5Q0J105k6m0J75R9J31L34j51kj2111K12J81r3145L76k32o9r0K06103
30b44k49L53J02Q7QK8j24k16J86k02J79J87m3K21k34k20L17j32J25N8117J61Nj86J26R4
4G0J71J43k15j18
0E1 $$ checkpoint
##END=
```

Example 3: An Example Peak Assignment.

```
##TITLE= Test Run 1001
##JCAMP-DX= 5.00
##DATA TYPE= NMR PEAK ASSIGNMENTS
##DATA CLASS= ASSIGNMENTS
##ORIGIN= Dr.J.Lambert, ISAS Dortmund, FRG
##OWNER= Copyright (C) 1992 by ISAS Dortmund, FRG
##.OBSERVE FREQUENCY= 100.4
##.OBSERVE NUCLEUS= ^13C
##SPECTROMETER/DATA SYSTEM= JEOL GX 400
##RESOLUTION= 1.470000
##XUNITS= PPM
##YUNITS= ARBITRARY UNITS
##NPOINTS= 22
##PEAK ASSIGNMENTS= (XYA)
(152.54, 1, (15))
(125.21, 1, (7))
(135.87, 1, (3))
...
##.COUPLING CONSTANTS= J(A,B)
8.500(5,18)
11.000(5,16)
165.300(3,19)
5.200(3,17)
...
##END=
```

Example 4: A Mask for a Compound File Consisting of Multiple DATA BLOCKS with Structure Data and NMR Peak Assignments.

All labeled data records (LDRs) not marked as OPTIONAL are REQUIRED
The text in ‘ ’ must be replaced by actual values.

```
##TITLE= 'title of the whole COMPOUND file'
##JCAMP-DX= 4.24 $$ 'Program, Version No.'
##DATA TYPE= LINK
##BLOCKS= 'n' $$ n is the number of the DATA BLOCKS
##ORIGIN= 'name of the contributor, organization, address, telephone'
##OWNER= COPYRIGHT (C) 'year' by 'name' $$ or PUBLIC DOMAIN

##TITLE= 'title of the first DATA BLOCK with structure data'
##JCAMP-CS= 3.7
##BLOCK_ID= 1
##ORIGIN= 'name of the contributor, organization, address, telephone'
##OWNER= COPYRIGHT (C) 'year' by 'name' $$ or PUBLIC DOMAIN
##CROSS REFERENCE= NMR PEAK ASSIGNMENTS:BLOCK_ID=2
... $$ structure info see Reference 4.
##END= $$ end of the first DATA BLOCK

##TITLE= 'title of the second DATA BLOCK with peak assignments'
##JCAMP-DX= 5.00
##DATA TYPE= NMR PEAK ASSIGNMENTS
##DATA CLASS= ASSIGNMENTS
##BLOCK_ID= 2
##ORIGIN= 'name of the contributor, organization, address, telephone'
##OWNER= COPYRIGHT (C) 'year' by 'name' $$ or PUBLIC DOMAIN
##OBSERVE FREQUENCY= 'frequency in MHz'
##OBSERVE NUCLEUS= '1H, 13C etc.'
##SOLVENT REFERENCE= 'solvent lock signal in ppm' $$ see 5.2.3/5.2.4
##DATE= 'YY/MM/DD' $$ OPTIONAL
##TIME= 'HH:MM:SS' $$ OPTIONAL
##SOURCE REFERENCE= 'your spectrum identification' $$ OPTIONAL
##CROSS REFERENCE= STRUCTURE:BLOCK_ID=1
                    $$ other associated block Ids
                    $$ e.g. INFRARED SPECTRUM:BLOCK_ID='m'
##SAMPLE DESCRIPTION= 'sample information' $$ OPTIONAL
                    $$ e.g. SOLVENT='solvent'
##NAMES= 'sample names' $$ OPTIONAL
##SPECTROMETER/DATA SYSTEM= 'spectrometer' $$ OPTIONAL
##TEMPERATURE= 'temperature in degrees C' $$ OPTIONAL
##XUNITS= 'HZ or PPM'
##YUNITS= ARBITRARY UNITS
##NPOINTS= 'number of the peak assignments'
##PEAK ASSIGNMENTS= (XYMA) $$ VARIABLE
                    ('x-value 1', 'y-value 1', 'multiplicity 1', ('assignment 1'))
                    ('x-value 2', 'y-value 2', 'multiplicity 2', ('assignment 2'))
...
##.COUPLING CONSTANTS= J(A,B) $$ OPTIONAL
                    'coupling constant 1' ('atom number 1', 'hetero-atom number 1')
                    'coupling constant 2' ('atom number 2', 'hetero-atom number 2')
...
##.RELAXATION TIMES= (XYR) $$ OPTIONAL
                    'x-value 1', 'y-value 1', 'relaxation time 1 in s'
                    'x-value 2', 'y-value 2', 'relaxation time 2 in s'
...
##END= $$ end of this DATA BLOCK
...
##END= $$ further structure and peak assignment blocks
##END=
##END= $$ end of the last DATA BLOCK
##END= $$ end of the COMPOUND JCAMP-DX FILE
```