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JCAMP-DX for EMR

(IUPAC RECOMMENDATIONS 2004)

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Abstract In this document, we define a data exchange format initially formulated from discussions of an INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY (IUPAC) limited term task group at the 35th Royal Society of Chemistry-ESR conference in Aberdeen 2002. The definition of this format is based on the IUPAC **J**oint **C**ommittee on **A**tomic and **M**olecular **P**hysical **D**ata **Ex**change (JCAMP-DX) protocols, which were developed for the exchange of infrared spectra [1] and extended to chemical structures [2], nuclear magnetic resonance data [3,4], mass spectra [5] and ion mobility spectra [6]. This standard of the JCAMP-DX was further extended to cover year 2000 compatible date strings and good laboratory practice [7] and the next release will cover the information needed for storing n-D data sets.[8]. The aim of this paper is to adapt JCAMP-DX to the special requirements for EMR, electron magnetic resonance.

1. INTRODUCTION

JCAMP-DX is an evolving, open-ended, machine-independent, self-documenting file format for exchanging and archiving data from computerized laboratory instruments like spectrometers, diffractometers, and others, whose output is commonly represented as spectral (profile) plots, contours, or peak tables. The first JCAMP-DX protocol was designed to meet the need for exchanging infrared spectra between similar instruments of different manufacturers. The present document is the result of ongoing efforts by users and manufacturers to extend JCAMP-DX to other types of instrumental data.

A major objective of JCAMP-DX is to enable routine capture of data at the source to make it available for exchange, archiving, and entry into databases. All data are represented as labelled fields of variable length using printable ASCII characters. A JCAMP-DX file is a text file which can be viewed, corrected, and annotated with ASCII text editors.

Use of the name JCAMP-DX to describe data files implies that they conform to the format and style described in the relevant protocols and the information content defined for a particular DATATYPE.

Use of the name JCAMP-DX in the description of software capability implies the ability to generate and read JCAMP-DX files as defined in the relevant published protocols for a particular DATATYPE (Section 4).

2. SIGNIFICANCE AND USE

This version of JCAMP-DX provides for a description of the file structure to be used to accommodate a very wide range of EMR applications.

Inasmuch as it is very desirable for instrument data systems to be able to read and write files in a standard format directly, instrument vendors are encouraged to develop JCAMP-DX software for the instruments which they currently support. It is feasible for vendors to do so for a tightly defined CORE of information.

3. BASIC STRUCTURE OF JCAMP-DX FILES.

JCAMP-DX is a FILE specification. The basic element of JCAMP-DX files is the LABELLED-DATA-RECORD (LDR). LABELLED-DATA-RECORDS are combined into BLOCKS. A FILE may contain more than one BLOCK.

A simple FILE would look like

```
Data Block          ##TITLE=
                            Headers
                            Data
                    ##END=
```

The BLOCK structure was first described for IR COMPOUND files in Section 11 of Reference 1.

```
Link Block          ##TITLE=
                            Define total number of BLOCKS
Data Block 1        ##TITLE=
```

```
                    ##END=
Data Block 2        ##TITLE=

                    ##END=
Data Block 3        ##TITLE=

                    ##END=
File End            ##END=
```

The NTUPLE structure was first described for NMR COMPLEX DATA STORAGE files in Section 7 of Reference 3.

```
                    ##TITLE=
                        Headers
                        ##NTUPLES=
                    ##PAGE=
                        Data
                    ##PAGE=
                        Data
                    ##END NTUPLES=
File End            ##END=
```

This is what we will normally mean by the word FILE.

The logical division of a JCAMP-DX file into CORE and NOTES subsets is a measure to separate the protocol for representing tabular data (CORE) which must be parsed by computer from that which is mainly for reference by humans.

4 CORE.

The CORE portion of a JCAMP-DX BLOCK or FILE is the irreducible minimum JCAMP-DX file. The CORE provides a focus for instrument and software vendors to convert between in-memory forms and JCAMP-DX. The CORE contains one or more data arrays, corresponding attributes for defining units, scale factors, sizes, etc., of arrays for the data, plus key application dependent attributes and identification. The main objective of the CORE is to focus on the information which must be transferred to a foreign system in order for it to process and/or plot and label the data as if it had been generated internally.

The CORE is divided into two subsets: CORE HEADER and CORE DATA.

4.1 CORE HEADER

The CORE HEADER provides for overall identification of a JCAMP-DX file. Each record is prefixed with a ## sign and represented as ##HEADER= in the BLOCK or FILE. For example, ##TITLE=My First EMR Spectrum
All the core headers are required elements. The CORE HEADER consists of:
TITLE,
JCAMP-DX,
DATATYPE,
DATA CLASS,
ORIGIN,
OWNER

In general information in the Header is either TEXT (free format) or STRING (reserved or predefined keywords) and information in the Data is either AFFN (ASCII FREE FORMAT NUMERIC) or ASDF (ASCII SQUEEZED DIFFERENCE FORM).

4.1.1 ##TITLE= (TEXT)

A description of the data file.

4.1.2 JCAMP-DX=(STRING) $$ for example JCAMP-DX _writer.exe version 0.99

The VERSION NUMBER of JCAMP-DX, followed by a comment on the version of the software writing the file.
(Required)

4.1.3 ##DATA TYPE= (STRING).

Electron Magnetic Resonance spectroscopy now includes a wide variety of techniques all of which involve measurements which exploit the magnetic properties or ascertain the environment of the unpaired electron. The description of many of these as either ESR, electron spin resonance, or as EPR, electron paramagnetic resonance is commonplace in the literature. However the great diversity of techniques now applied to the measurement of paramagnetism, usually (but not always) in the presence of an external magnetic field, needs a generic descriptive term. In particular the emergence of imaging technology, of techniques such as ENDOR which sits between NMR and EPR/ESR, and of newer optical detection techniques, leads us to suggest an overall classification as 'EMR'. The use of the *historical* terms ESR or EPR thus falls under this overall classification, a situation which we do not wish to change. *(The present IUPAC recommendation is to use the term EPR rather than ESR?)* The task group has therefore decided to adopt the generic title for the DATA TYPE as EMR, and to define all the METHODs in terms of either a MEASUREMENT or a SIMULATION.
e.g. ##DATA TYPE= EMR MEASUREMENT

e.g. ##DATA TYPE= EMR SIMULATION
(Required)

4.1.4.##DATA CLASS= (STRING).
This LDR contains the name of the type of tabular data, i.e., XYDATA, XYPOINTS, PEAK TABLE, PEAK ASSIGNMENTS, BLOCKS, or NTUPLES. Coates [9] first pointed out that the data for a number of different applications (IR and Raman spectra, GC retention times and NMR Chemical Shift) are so similar that JCAMP-DX files for all these types can be plotted or processed (smoothed, peak-picked, deconvoluted, etc.) by existing software for one of the techniques. This can clearly be extended to many other types to XY data which are represented in the XYDATA form, and probably also as XYPOINTS.

##DATA CLASS= is intended to provide an early indication to software for the purpose of determining whether or not it can process a given file. This seems important because it allows crossover of data processing routines between different techniques
(Required)

4.1.5 ##ORIGIN=(TEXT)

The origin of the data, i.e. the name of the organisation.
(Required)

4.1.6 ##OWNER=(TEXT)

The owner or author of the data. This can be “public domain” or the name of the person or organisation and may include a copyright note.
(Required)

4.2 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 electron magnetic resonance. However, in the case of the equipment parameters, the particular requirements of this technique call for some special LDRs. In the following part, definitions are given for LDRs that will allow a precise description of the equipment parameters for all EMR experiments (Note the syntax of ##.LABEL=.)

4.2.1 ##.DETECTION MODE= CW or PULSE *(required)*

4.2.1.1 CW
Continuous wave, the frequency (or field) dependence of the sample is measured in response to a periodic perturbation of microwave radiation to the sample.

4.2.1.2 PULSE
One or more pulses of (e.g. microwave and/or RF) radiation are used to perturb the sample, and the recovery from this perturbation is measured as a function of a swept variable.

CW and pulse measurements are related via the Fourier Transform [10,11,12].
.
(Required)

4.2.2 ##.METHOD= (STRING)
There are a wide variety of experimental methods used in EMR. The acronyms used are those described in the references used for the DETECTION MODE. The protocol description in this document concerns the following.

Abbreviations associated with other forms of EMR measurements not mentioned above, and which may need inclusion in the METHOD LDR in the future. Some of these will require extra EMR specific LDRs, but some may use the present set. Since many of these use pulse excitation, they will require methods to define pulse sequences.

ADMR – absorption detected magnetic resonance
CIDEP – chemically induced dynamic electron polarization
COSY – 2D correlation spectroscopy
CYCLOPS – cyclically ordered phase sequence
DECENT – decoupled ESEEM correlated to nuclear transition frequencies
DEER – double electron electron resonance
DEFENCE – deadtime free ESEEM by nuclear coherence-transfer echoes
DONUT – double nuclear coherence transfer
ELDOR – Electron-electron double resonance
EPR – electron paramagnetic resonance (encompassed by SPECTRUM)
ESR – electron spin resonance (encompassed by SPECTRUM)
ESR-STM ESR scanning tunnelling microscope
ESE – electron spin envelope field sweep spectroscopy
ESEEM – electron spin echo envelope modulation
EXSCY (EXSY) – two dimensional exchange spectroscopy
FDMR – fluorescence detected magnetic resonance
FMR – very high field EPR
FORTE – forbidden-transition labelled EPR

HETEROCOSY – nD correlation spectroscopy
HFEPR – high field EPR
HYEND – hyperfine correlated ENDOR
HYSCORE – hyperfine sublevel correlation spectroscopy
LEFE – linear electric field effect
LODESR – longitudinal-detected ESR
LOD-PEPR – longitudinal-detected pulsed EPR
LOD-ESEEM - longitudinal-detected ESEEM
LOMENDOR – longitudinally modulated ENDOR
MARY – magnetic field dependence of (effect on) reaction yield
MAS-EPR – magic angle spinning EPR
MODR – microwave optical double resonance
MQ-EPR – multiple quantum EPR
MQ-ELDOR – multiple quantum ELDOR
MQ-ENDOR – multiple quantum ENDOR
NZ-ESEEM - nuclear-Zeeman-Resolved ESEEM
PCDMR – photoconductive detected magnetic resonance
PEANUT – phase inverted echo-amplitude detected nutation
PEDRI – proton-electron double resonance imaging
PYESR – product yield detected ESR
RAS-EPR – right-angle spinning EPR
RYDMR – reaction yield detected magnetic resonance
SECSY – spin-echo correlated spectroscopy
SEDOR – spin-echo double resonance
SEESR – simultaneous electrochemistry ESR
SIFTER – single frequency technique for refocusing
SMART – single pulse matched resonance transfer
TREPR – time-resolved EPR
TRFDMR – time resolved fluorescence detected magnetic resonance

The list is intended to be as complete as possible to allow researchers to classify their particular form of spectrum. However, a number of the abbreviations are already encompassed by the current METHODs.
One possible route for defining these abbreviations might be by using a JCAMP-DX private LDR. Users can devise their own private labels to cover items they wish to include in the data file for completeness, e.g. ##$RYDMR. Note however, that many software packages do not parse private labels and they may not be rewritten if saved from within an application.
{If used, the abbreviations need to have references}

4.2.2.1 DYNAMIC

Any of a number of electron magnetic resonance experiments in which a non-Boltzmann spin state distribution is produced by a combination of radical pairs or directly from the triplet state.

4.2.2.2 ELDOR

Electron-Electron DOuble Resonance is a technique in which one frequency is used to pump an electronic transition at one frequency while observing at another frequency. It is often used to determine distances between centers containing unpaired electrons in different environments.

4.2.2.3 ENDOR

Electron-Nuclear Double Resonance has been described as EMR detected NMR and makes use of electron-nuclear hyperfine couplings between unpaired electrons and neighbouring nuclei.

4.2.2.4 ESEEM

Electron Spin Echo Envelope Modulation is a pulsed technique used for observing solid phase samples. [13]

4.2.2.5 ODMR

Any EMR experiment in which spin transition are detected by optical means.

4.2.2.6 GONIOMETER

Any EMR experiment in which sample angle relative to the main magnetic field is one of the axes.

4.2.2.7 HYSCORE

The Hyperfine Sublevel Correlation Spectroscopy sequence was introduced in 1986 as a two-dimensional four pulse experiment [14].

4.2.2.8 KINETIC

Any EMR experiment in which time is one of the axes.

4.2.2.9 SATURATION

Any EMR experiment in which microwave power is one of the axes.

4.2.2.10 SPECTRUM

Any EMR experiment in which the magnetic field is one of the axes.

4.2.2.11 FID

Any EMR experiment in which the free induction decay is detected.

4.2.2.12 TRIPLE

Any EMR experiment, which involves the use two RF fields for modulating nuclear spins.

4.2.2.13 IMAGING

Any EMR experiment in which distance is one or more of the experimental axes.

4.2.2.14 SPECTRAL SPATIAL

Any EMR experiment in which distance and magnetic field are the experimental axes.
(METHOD is *Required*)

4.2.3 ##.DETECTION METHOD= (TEXT)

Used where a resonator is not involved in the measurement and can name e.g. fluorescence, phosphorescence, photoconductivity, reaction yield. An alternative where appropriate is to give a wavelength for the detector, this may be applicable for HFEPR.

4.2.4 ##.MICROWAVE FREQUENCY1= (AFFN)

Typical EMR experiments were conducted at a fixed microwave frequency ranged from few MHz to hundreds of GHz. To accommodate EMR experiments that utilized more than one source of microwave radiation, the number 1 and 2 are appended to the LDRs. The microwave frequency is expressed in Hz.

4.2.5 ##.MICROWAVE POWER1= (AFFN)

The power of microwave source in watts.

4.2.6 ##.MICROWAVE PHASE1= (AFFN)

The phase of the microwave source in degrees.

4.2.7 ##.MICROWAVE FREQUENCY2= (AFFN)

The frequency for the second microwave source in Hz. (Required for ELDOR)

4.2.8 ##.MICROWAVE POWER2= (AFFN)

The power for the second microwave source in watts. (Required for ELDOR)

4.2.9 ##.MICROWAVE PHASE2= (AFFN)

The phase for the second microwave source in degrees. (Required for ELDOR)

4.2.10 ##.RECEIVER GAIN= (AFFN)

A scalar factor (gain) that is applied to the detection signal.

4.2.11 ##.MODULATION UNIT= (TEXT)

In a typical CW EMR experiment, the signal can be modulated by either field or frequency to achieve the enhancement of the signal resolution. The source of the modulation must be specified. (Required for CW)

4.2.12 ##.MODULATION AMPLITUDE= (AFFN)

The amplitude of the corresponding modulation unit. For example, the amplitude of field modulation is kept small compared to the linewidth in order to avoid over saturation of the signal. (Required for CW)

4.2.13 ##.MODULATION FREQUENCY= (AFFN)

The frequency of modulation unit. The typical used modulation frequency in an EMR experiment is 100 KHz. (Required for CW)

4.2.14 ##.RECEIVER HARMONIC= (AFFN)

The typical CW experiment is recorded in 1st harmonic (i.e. ##. RECEIVER HARMONIC=1). However, it can also be recorded as 2nd or 3rd Harmonics. (Required for CW)

4.2.15 ##.DETECTION PHASE= (AFFN)

The common used technique for EMR experiments is the phase-sensitive detection and is often calibrated to 0 degree relative to the reference arm. Therefore, the phase of the detector must be reported especially when the spectrum is not recorded in phase. (Required for CW)

4.2.16 ##.SCAN TIME= (AFFN)

The time (in seconds) required to complete one scan of the spectrum.

4.2.17 ##.NUMBER OF SCANS= (AFFN)

The total number of scans for a spectrum. (1 if a single scan)

4.2.18 ##.GONIOMETER ANGLE= (AFFN)

Assumes a single circle goniometer. The crystal orientation will also need to be recorded as will the crystal structure properties of the host lattice, and assuming the measurements are on a magnetically dilute sample chemical details of the host will be needed. (Required if .METHOD=GONIOMETER)

4.2.19 ##.STATIC FIELD= (AFFN)

The static magnetic field in Gauss. This is commonly used when carry out double resonance or spin echo experiments. (Required for ENDOR)

4.2.20 ##.SCANNED RF POWER= (AFFN)

In a double resonance experiment, say ENDOR, a constant power of RF source was used to scan for nuclear transitions. (Required for ENDOR)

4.2.21 ##.PUMPED RF FREQUENCY 1= (AFFN)

In a double resonance experiment, say ENDOR, this is the frequency of the RF source which was used to scan for nuclear transitions (units are in Hz). (Required for TRIPLE)

4.2.22 ##.PUMPED RF POWER 1= (AFFN)

In a double resonance experiment, say ENDOR, this is the power of the RF source which was used to scan for nuclear transitions (units are in Watts). (Required for TRIPLE)

4.2.23 ##.GRADIENT THETA= (AFFN)
For EMR imaging experiments, this is the intensity of the gradient magnetic field along the theta angle (using spherical coordinates - units are in Tesla). (Required for IMAGING)

4.2.24 ##.GRADIENT PHI= (AFFN)

For EMR imaging experiments, this is the intensity of the gradient magnetic field along the phi angle (using spherical coordinates - units are in Tesla). (Required for IMAGING)

4.2.25 ##.GRADIENT STRENGTH IN THETA/PHI DIRECTION= (AFFN)
For EMR imaging experiments, this is the intensity of the total angular gradient magnetic field (using spherical coordinates - units are in Tesla) (Required for IMAGING)

4.2.26 ##.GRADIENT STRENGTH X= (AFFN)
For EMR imaging experiments, this is the intensity of the gradient magnetic field along the X axis (units are in Tesla). (Required for IMAGING)

4.2.27 ##.GRADIENT STRENGTH Y= (AFFN)
For EMR imaging experiments, this is the intensity of the gradient magnetic field along the Y axis (units are in Tesla). (Required for IMAGING)

4.2.28 ##.GRADIENT STRENGTH Z= (AFFN)
For EMR imaging experiments, this is the intensity of the gradient magnetic field along the Z axis (units are in Tesla). (Required for IMAGING)

4.2.29 ##.SIMULATION SOURCE= (TEXT)

The sources or tools used to simulate the spectrum (e.g. QPOW, Bruker, WinEPR, etc.). (Required for EMR SIMULATION)

4.2.30 ##.SIMULATION PARAMETERS= (TEXT)

The detailed descriptions of the EMR parameters that are needed to reproduce the simulated spectra such as microwave frequency, hyperfine coupling constants, rotation angles, static magnetic fields, scan range, linewidth, etc. (Required for EMR SIMULATION)

4.3 CORE DATA

4.3.1 ##XUNITS= (STRING) and ##YUNITS= (STRING)
Here, the units of the axes can be given as one of the following keywords:
For ##XUNITS=: DEGREES, HERTZ, KELVIN, SECONDS, TESLA, WATTS.
For ##YUNITS=: POWER, INTENSITY and ARBITRARY UNITS.
(Required)

4.3.2 ##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)

4.3.3 ##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)

4.3.4 ##XFACTOR= (AFFN) and ##YFACTOR= (AFFN)
The values of a spectrum may be converted to integer to save space and allow the DIFDUP format (see [1] Section 5). 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 larger scaling is necessary, it is required to give the actual unscaled maximum and minimum of the ordinates in the records ##MAXY= and ##MINY=.
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.
(*Required for ASDF data types. Should be to 1.0 for AFFN*)

4.3.5 ##NPOINTS= (AFFN)
The number of points in the data table is required for all data classes: XYDATA, XYPOINTS, PEAK TABLE, and PEAK ASSIGNMENTS.
(Required, handled by VAR_DIM in NTUPLE files)

4.4 CORE DATA TABLE

Data must be stored in one of the following data formats (Sections 4.4.1–4.4.4). 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.

4.4.1 ##XYDATA= (AFFN or ASDF).
This LDR contains a table of spectral data with abscissa values at equal intervals specified by parameters defined in Section 4.3. 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 points, 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 ASDF forms defined in JCAMP-DX 4.24 (Reference 1)

produce much smaller files but at the cost of reduced human readability. In modern computers systems file size is no longer the restriction it used to be and the task group felt that users may be more comfortable with AFFN which would also allow the storage of numbers in scientific notation.

4.4.2 ##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. For example, X1, Y1; X2,Y2, …, Xi, Yi.

4.4.3 ##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 semicolon or space, components of a group are separated by commas.

4.4.4 ##PEAK ASSIGNMENTS= (STRING)
Variable list: (XA), (XYA), or (XYWA)
After this LDR, a list of peaks and their assignments for each component is given in the following form:
(X1, [Y1, [W1]], <A1>)
. . . .
(Xi, [Yi, [Wi]], <Ai>)
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.

5. 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 employed in the experiment.

5.1 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 [1–6].
At least one of the optional LDRs described in Sections 5.1.3–5.1.8 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.

5.1.1 ##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)

5.1.2 ##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)

5.1.3 ##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)

5.1.4 ##IUPAC NAME=(STRING)
The use of IUPAC names for the sample has been recommended previously by the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division in 1991.
(Optional)

5.1.5 ##CAS NAME= (STRING)

Sample 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)

5.1.6 ##NAMES= (STRING)
Here, the common, trade, or other names are allowed. Multiple names are placed on separate lines.
(Optional)

5.1.7 ##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 and are terminated by the next nondigit. The 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.
Examples:
C2H4O2 or C2 H4 O2 (ethanoic acid)
H2 /\17O (water, mass 17 oxygen)
(Optional)

5.1.8 ##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)
(N1, C1, U1)
. . .
(Ni, Ci, Ui)
The group for each component is enclosed in parentheses. Each group starts a new line and may continue on following lines.
(Optional)

5.1.9 ##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)

5.1.10 ##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)

5.1.11 ##XLABEL= (TEXT) and ##YLABEL= (TEXT)
These LDRs give the possibility of labeling the axes.
(Optional)

5.1.12 ##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 the Y-range exceeds recommended ordinate scaling (Section 4.3.4).
(Optional)

5.2 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., ##**.**MICROWAVE FREQUENCY=). 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., ##EMR MEASURMENT**.**MICROWAVE FREQUENCY=.

5.2.1 ##.RESONATOR= (TEXT)

In a typical EMR spectrometer the resonator (a.k.a. cavity) is used to hold the sample, however a resonant cavity is not required to achieve resonance (!). This LDR enables the cavity to be described, e.g. TE_{102} rectangular, TE_{011} cylindrical, helical, loop-gap, Fabry-Perot

5.2.2 ##.TIME CONSTANT= (AFFN)

This is most appropriate with legacy measurements where a signal was measured and recorded on a chart recorder. With digital recording, especially where an integrating ADC is used, the interpretation of a time constant is problematic. The time constant is an output filter that utilizes resistive-capacitive filter to filter the output of the phase-sensitive detector to improve the signal to noise. The time constant is expressed in seconds.

5.2.3 ##.PUMPED RF FREQUENCY 2= (AFFN)

In a triple resonance experiment, this is the frequency of the RF source which was used for the third source (units are in Hz).

5.2.4 ##.PUMPED RF POWER 2= (AFFN)

In a triple resonance experiment, this is the power of the RF source which was used for the third source (units are in Watts).

5.2.5 ##DATA PROCESSING= (TEXT)

The descriptions of methods or algorithms used to process the data (e.g. FT).

5.2.6 ##.CALIBRATION STANDARD= (TEXT)

The chemical standard used internally or externally to calibrate the g value of an EMR signal. (e.g. DPPH or MgO_2).

5.2.7 ##.X_OFFSET= (AFFN)

The numerical offset of the global X axis.

6. SUMMARY

The following table lists the LDRs discussed with their basic parameters shown.

Table 1. Relevant terms for EMR

Parameter	**Allowable words and UNITS**	**Comments**
##TITLE=	TEXT	REQUIRED
##JCAMP-DX=	5.01 STRING	REQUIRED
##DATA TYPE=	EMR MEASUREMENT, EMR SIMULATION	REQUIRED
##DATA CLASS=	XYDATA, XYPOINTS, PEAK TABLE or ASSIGNMENTS	REQUIRED
##ORIGIN=	TEXT	REQUIRED
##OWNER=	TEXT	REQUIRED
##LONGDATE=	YYYY/MM/DD [HH:MM:SSSS[.SSSS][±UUUU]]	OPTIONAL
##SPECTROMETER/DATA SYSTEM=	TEXT	OPTIONAL
##.DETECTION MODE=	CW, PULSE	REQUIRED
##.METHOD=	DYNAMIC, ELDOR, ENDOR,ESEEM, ODMR, GONIOMETER, HYSCORE, KINETIC, SATURATION, SPECTRUM, FID, TRIPLE, IMAGING, SPECTRAL SPATIAL, STRING	REQUIRED

##.RESONATOR=	TEXT	OPTIONAL
##.MICROWAVE FREQUENCY1=	HERTZ	REQUIRED
##.MICROWAVE POWER1=	WATT	REQUIRED
##.MICROWAVE PHASE1=	DEGREES	REQUIRED
##.MICROWAVE FREQUENCY2=	HERTZ	REQUIRED for ELDOR
##.MICROWAVE POWER2=	WATT	REQUIRED for ELDOR
##.MICROWAVE PHASE2=	DEGREES	REQUIRED for ELDOR
##.RECEIVER GAIN=	DIMENSIONLESS NUMBER	REQUIRED
##.MODULATION UNIT=	TESLA, HERTZ, LUMENS, STRING	REQUIRED for CW
##.MODULATION AMPLITUDE=	NUMBER, IN UNITS OF MODULATION UNIT	REQUIRED for CW
##.MODULATION FREQUENCY=	HERTZ	REQUIRED for CW
##.RECEIVER HARMONIC=	POSITIVE INTEGER, usually 1	REQUIRED for CW
##.DETECTION PHASE=	DEGREES	REQUIRED for CW
##.TIME CONSTANT=	SECONDS	OPTIONAL
##.SCAN TIME=	SECONDS	REQUIRED
##.NUMBER OF SCANS=	INTEGER	REQUIRED
##.GONIOMETER ANGLE=	DEGREES	REQD if .METHOD= GONIOMETER
##.STATIC FIELD=	TESLA	REQUIRED for ENDOR
##.SCANNED RF POWER=	WATTS	REQUIRED for ENDOR
##.PUMPED RF FREQUENCY 1=	HERTZ	REQUIRED for TRIPLE
##.PUMPED RF POWER 1=	WATTS	REQUIRED for TRIPLE
##.PUMPED RF FREQUENCY 2=	HERTZ	OPTIONAL for TRIPLE
##.PUMPED RF POWER 2=	WATTS	OPTIONAL for TRIPLE
##DATA PROCESSING=	TEXT	OPTIONAL
##.CALIBRATION STANDARD=	TEXT	OPTIONAL
##.X_OFFSET=	NUMBER	
##.GRADIENT THETA=	TEXT, DEGREES	REQUIRED for IMAGING
##.GRADIENT PHI=	TEXT, DEGREES	REQUIRED for IMAGING
##.GRADIENT STRENGTH IN THETA/PHI DIRECTION=	TEXT, T/M	REQUIRED for IMAGING
##.GRADIENT STRENGTH X=	TEXT, T/M	REQUIRED for IMAGING
##.GRADIENT STRENGTH Y=	TEXT, T/M	REQUIRED for IMAGING

##.GRADIENT STRENGTH Z=	TEXT, T/M	REQUIRED for IMAGING
##.SIMULATION SOURCE=	TEXT	REQUIRED FOR EMR SIMULATION
##.SIMULATION PARAMETERS=	TEXT	REQUIRED FOR EMR SIMULATION
##SAMPLE DESCRIPTION=	TEXT	OPTIONAL
##CAS NAME=	TEXT	OPTIONAL
##STATE=	Solid, liquid, gas, etc. TEXT	OPTIONAL
##CONCENTRATION=	TEXT	OPTIONAL
##XUNITS=	DEGREES, HERTZ, KELVIN, SECONDS, TESLA, WATTS, STRING	to be used as XLABEL if ##XLABEL is undefined. REQUIRED
##YUNITS=	PREDEFINED, can be ARBITRARY UNITS, STRING	REQUIRED
##XLABEL=	FIELD, TIME, ANGLE, TEMPERATURE, POWER, TEXT	OPTIONAL
##XFACTOR=	NUMBER	= 1 if no compression
##YFACTOR=	NUMBER	= 1 if no compression
##FIRSTX=	NUMBER	REQUIRED for XYDATA
##LASTX=	NUMBER	REQUIRED for XYDATA
##NPOINTS=	POSITIVE INTEGER	REQUIRED
##FIRSTY=	NUMBER	REQUIRED
##$NOTES	TEXT	from legacy data
##END=		REQUIRED

Example files

```
##TITLE= Toluene soln : D. trapped by Phenyl-t-butylnitrone(PBN)
##JCAMP-DX=  5.01   $$ Manual conversion from Bruker file
##DATA TYPE= EMR SPECTRUM
##DATA CLASS= XYDATA
##ORIGIN= School of Chemistry , University of Bristol
##OWNER= John Maher : john.maher@bristol.ac.uk
##DATE= 2000/11/26
##SPECTROMETER/DATA SYSTEM= Bruker ESP300E
##.DETECTION MODE= CW
##.METHOD=  ESR
##INSTRUMENTAL PARAMETERS= X Band
##.FREQUENCY= 9.7667680GHz
##.POWER= 20.0 mW
##.GAIN= 1.0E4
##.MODULATION FREQUENCY= 100kHz
##.MODULATION AMPLITUDE= 1.015G
##.CENTRE= 0.3472016
##.SWEEP= 0.0059990
##DELTAX=   .4885179E-05
##XUNITS= TESLA
##YUNITS= INTENSITY
##XFACTOR=   .1068751E-4
##YFACTOR=   .2414014E-01
##FIRSTX=   0.3441986
##LASTX=   0.3501976
##MAXY=   791.0000
##MINY=  -786.0000
##NPOINTS=   1229
##FIRSTY=  -4.000000
##XYDATA=(X++(Y..Y))
32206a66k07K07J66j24k07j66Q3J65J25m2j65%J65J66Q3k07p04r95q28l73K49P87R94T
32217@P46N80L31M1k48m56m97Tl31k08%J25K90L31M56K07q3m14l73q3Q3K90L31J66j66
32228F21m97o21m97j66L32M97M55K49m2j65j66Tm1M1K07K90K08k08p04j118j077m56K90
32239b734Q70R53O62K08j25j65j66%Q3K07J24Q3M1M2M1q3m1%Vm1j25M2J24L73TJ24k07
32252F63l73k90%K49L31K48m1k90m97l73l31j24Q2K49L31K49J24%m1j25m1q3m14o21o227.
…..
…..
32757a24K90Q28Q29M97m2m97p45o63l73j24M1Q3J66J24j24k07m56k90m1K48J24
32767d56
##END=
```

7. ACKNOWLEDGEMENTS

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8. REFERENCES

1. R. S. McDonald and P. A. Wilks Jr. "JCAMP-DX: A Standard Form for Exchange of Infrared Spectra in Computer Readable Form", *Appl. Spectrosc*. **42**, 151–162 (1988) and "JCAMP-DX. A standard format for the exchange of infrared spectra in computer readable format (IUPAC Recommendations 1991)", *Pure Appl. Chem*. **63**, 1781–1792 (1991).

2. J. Gasteiger, B. M. P. Hendriks, P. Hoever, C. Jochum, H. Somberg. "JCAMP-CS: A Standard Exchange Format for Chemical Structure Information in Computer-Readable Form", *Appl. Spectrosc.* **45**, 4–11 (1991)
.

3. A. N. Davies and P. Lampen. "JCAMP-DX for NMR", *Appl. Spectrosc.* **47**, 1093–1099 (1993).

4. A.N. Davies, J. Lambert, R.J. Lancashire, P. Lampen with W. Conover, M. Frey, M. Grzonka, E. Williams, and D. Meinhart, "Guidelines for the Representation of Pulse Sequences for Solution-State Nuclear Magnetic Resonance Spectrometry (IUPAC Recommendations 2001)" *Pure Appl. Chem.*, **73**, 1749-1764, (2001).

5. P. Lampen, H. Hillig, A. N. Davies, M. Linscheid. "JCAMP-DX for Mass Spectrometry", *Appl. Spectrosc.* **48**, 1545-1552 (1994).

6. J.I. Baumbach, P. Lampen, A.N. Davies. "IUPAC/JCAMP-DX. An International Standard for the Exchange of Ion Mobility Spectrometry Data", Pure & Appl. Chem., Vol. 73, No. 11, pp. 1765-1782, 2001.

7. P. Lampen, J. Lambert, R. J. Lancashire, R. S. McDonald, P. S. McIntyre, D. N. Rutledge, T. Fröhlich, A. N. Davies. "An Extension to the JCAMP-DX Standard File Format, JCAMP-DX V.5.01 (IUPAC Recommendations 1999)", *Pure Appl. Chem.* **71**, 1549–1556 (1999).

8. for a draft, see http://www.jcamp.org

9. J.P. Coates, "Computers in Spectroscopy Part 3", *Spectroscopy*, **2**, 14-18, 120-22, (1987).

10. "Electron Paramagnetic Resonance", J.A.Weil, J.R.Bolton, J.E.Wertz, Wiley-Interscience, 1994. ISBN 0 471 57234 9

11: “Principles of pulse electron paramagnetic resonance”, A.Schweiger and G.Jeschke, Oxford U.P., 2001. ISBN 0 19 850634 1

12. “Morden pulsed and continuous-wave electron spin resonance” edit by Larry Kevan and Michael Bowman, John Wiley & Sons, New York, ISBN 0-471-50274-X.

13. L.G. Rowan, E.L. Hahn and W. B. Mims, "Electron spin echo envelope modulation", Phys. Rev. A, 137, 61 (1965).

14. P. Hoefer, A. Grupp, H. Nebenfuehr, and M. Mehring, "Hyperfine sublevel correlation (HYSCORE) spectroscopy: a 2D ESR investigation of the squaric acid radical", Chem. Phys. Lett. 132, 279 (1986).