
JCAMP-DX Spectral File Format for Submissions to the Infrared & Raman Users Group (IRUG) Database

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Abstract. This paper presents guidelines for the submission of spectra in the JCAMP-DX format to the IRUG (*Infrared and Raman Users Group*) Database. JCAMP-DX was chosen as the file format as it is platform independent and will allow error-free transfer of spectral information between various instruments and users. IRUG will use the JCAMP-DX files as the principal source of information for submitted spectra. All information pertaining to the sample and spectrum (as outlined on the IRUG Spectrum Submission Form) is incorporated into the JCAMP-DX file in a consistent format to create a complete data record. This format, consisting of both JCAMP-DX 4.24 and user (IRUG) defined Labelled-data-records (LDRs), is described. The LDRs for IRUG have been kept to a minimum to facilitate automatic transfer of the information when the IRUG JCAMP-DX files are imported into the users' infrared software packages.

1. Introduction

JCAMP-DX files are non-proprietary ASCII text files, developed by the *Joint Committee on Atomic and Molecular Physical Data* [1] to allow transfer of spectral information between different instruments and different users. The files can be read and edited using standard text editors (such as WordPad[®] or Notepad[®]) and are compatible to varying degrees with most commercial IR software packages. JCAMP-DX files consist of descriptive information (title, JCAMP version, data type, origin of data, instrument, sampling, sample details, etc.) in addition to the spectral data. JCAMP-DX was chosen as the file format for submission of spectra to the ***Infrared and Raman Users Group (IRUG) Database*** as it is platform independent and should allow error-free transfer of spectral information between various instruments and users. IRUG will use the JCAMP-DX files as the primary information source for all spectra in the database. All information pertaining to the sample and spectrum must be incorporated into the JCAMP-DX file in a consistent format. This paper details how descriptive information is directly inserted into the JCAMP-DX file using both JCAMP-DX 4.24 and a limited number of user (IRUG) defined *labelled-data-records* to assemble a complete IRUG formatted JCAMP-DX file for each spectrum.

2. Background: the JCAMP-DX Format for IRUG Submissions

The **IRUG Spectrum Submission Form** and **Numerical Key** (pages 6 and 7) list the information to accompany spectra submitted to the IRUG database. Acronyms for institutions are listed in **Institution Acronym Key** (pages 16 and 17). Most of this information is not automatically inserted into a native (proprietary) spectral file when it is acquired using commercial instrument IR software. To insert / restore the missing information, the user must manually edit the JCAMP-DX file after it has been created.

Format and Content

A JCAMP-DX file consists of a series of linked *labelled-data records (fields)* known as *LDRs*. Each LDR is one or more lines in an ASCII file beginning with a *data label name (label)* followed by corresponding information and data [1].

Column A of the **IRUG Guidelines for JCAMP-DX Files** (pages 8 - 13) lists the labels required by IRUG. There are two types of labels: *JCAMP-DX 4.24* and *IRUG*. The JCAMP labels are recognized in a file by the prefix **##** and are defined by JCAMP. Many are automatically inserted into the native file during conversion but must be edited when storing additional information from the IRUG submission form. **##TITLE=** is an example of a JCAMP defined label. IRUG labels are denoted by the prefix **##\$**. These are known as “user” defined labels and were developed by IRUG to store information for which there is no pre-existing JCAMP label. Since IRUG labels are not automatically generated, these must be both inserted and edited by the user. There are a total of eight IRUG labels: **##\$Material Source=**, **##\$Source Location=**, **##\$Sample Identifier=**, **##\$Colour=**, **##\$Age=**, **##\$Institution File Name=**, **##\$IRUG Material Class=**, and **##\$License=**.

Column C of the **Guidelines** lists the corresponding information/data required for each label as defined by JCAMP [2]. These JCAMP requirements have been modified by IRUG and resulting IRUG definitions are listed in Column B. To simplify the creation of IRUG formatted JCAMP files, the **General Format for IRUG Infrared JCAMP-DX Files** and the **General Format for IRUG Raman JCAMP-DX Files**, have been developed as user templates (pages 14 and 15) and examples of spectral files in the **General Format** are found on pages 18 to 20.

Order of LDRs

For a JCAMP file to function properly, the first three LDRs must always be in the order of **##TITLE=**, **##JCAMP-DX=**, **##DATA TYPE=**. It is also necessary for the final LDR to be **##END=**. The order of the remaining LDRs is not critical and various JCAMP converters may order the LDRs differently (compare examples on pages 18 to 20). For convenience, IRUG has grouped the LDRs as follows: compulsory (title, JCAMP version, data type), submitting institution details, instrument details, sampling details, sample details, additional IRUG sample details, and spectral information.

Characters per Line Limit

Lines in the JCAMP file must not exceed a total of 80 characters (including the label). This ensures that lines are not truncated when data are imported and that the file will open properly. Where necessary, entries for labels (except the first label, ##TITLE=) can be split over multiple lines by continuing the entry on the next line (see page 19, Example 2B, ##SAMPLING PROCEDURE). Since 17 spaces in the first or title line are reserved for the label and IRUG file name, a maximum of 63 characters remain for file description.

Appearance and consistency

For consistency in appearance, the format for the title should be: the filename followed by a space, then the material name with an initial capital letter. The remaining entries on the title line should be lower case, except for proper names and the institution acronym, and should be separated by commas. To minimize compatibility issues between different spectral software, infrared files should be converted to absorbance. Apart from title entries, multiple data entries in a single field should be separated by semicolons.

Optional LDRs

Some LDRs are optional; data for these labels may not be available or applicable (see page 19, Example 2B, ##PATHLENGTH, ##PRESSURE, ##TEMPERATURE, etc). If there is no information to enter, the square brackets enclosing generic text should remain as shown in the **General Format for IRUG JCAMP-DX Files** on pages 14 and 15)

Duplicate Information

In some cases, information is entered in more than one LDR to satisfy the JCAMP definitions (see page 19, Example 2B, ##SAMPLE DESCRIPTION= and ##SAMPLING PROCEDURE=).

3. How to Edit the JCAMP-DX file

The general procedure for creating a complete IRUG formatted JCAMP-DX 4.24 file from a native infrared file is as follows:

1. Convert the native infrared file (Perkin Elmer, Nicolet, Analect, etc. format) in **absorbance** using a JCAMP converter (spectrometer manufacturer's software, GRAMS32[®], or other software) to JCAMP-DX format.
2. Open the converted JCAMP-DX file in a text editor such as WordPad or Notepad. The converted file will resemble Examples 1A - 3A shown on pages 18 to 20.
3. Edit the JCAMP-DX file following the **General Format for IRUG JCAMP-DX Files** (page 14 or 15):
Insert any missing JCAMP-DX labels and the eight IRUG defined labels (##\$License=, ##\$Institution File Name=, ##\$Material Source=, ##\$Source

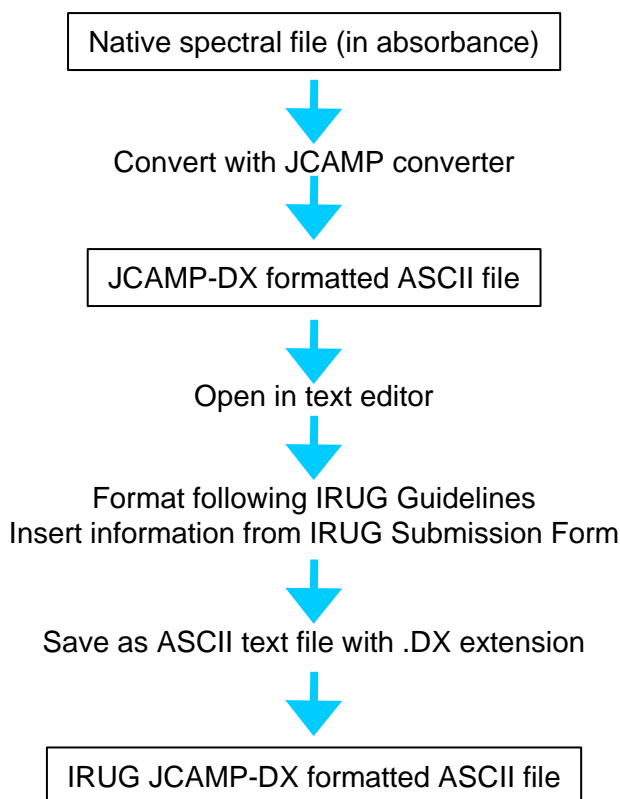
Location=, ##\$Sample Identifier=, ##\$Colour=, ##\$Age=, and ##\$IRUG Material Class=) before ##XUNITS=.

Insert the information listed on the IRUG Spectral Submission Form after the appropriate labels. Complete as many the LDR fields as possible. Be mindful of 80-character line limit; continue entries in excess of 80 characters on consecutive lines. The edited file should resemble Examples 1B - 3B shown pages 18 to 20.

4. Save the new JCAMP-DX file as an **ASCII text file** with the DX extension (NAME.DX). Check that the new file will open in your spectrometer's software.
5. **CAUTION: do not overwrite** the newly edited JCAMP-DX files with files from the original manufacturer's operating software (or JCAMP-DX converter software) as the changes/additions made in WordPad or Notepad will be overwritten and lost.

IRUG formatted Raman files are edited in a similar manner but the ordinate axis units should be **relative intensity**.

Editing procedure summary



4. Summary

A uniform, platform-independent format based on JCAMP-DX has been adopted for spectra submitted to the **Infrared and Raman Users Group (IRUG) Database**. The format uses combined JCAMP-DX 4.24 and IRUG defined labels for labelled-data-records (LDRs) that will accommodate the information requested for spectral submissions to the **IRUG Database**. The use of all labels, insofar as possible, will ensure that all pertinent information is contained within the JCAMP-DX file, creating a complete data record for each spectrum. The result is data of improved quality, and an **IRUG Database** that may be treated as a primary reference.

5. References

- 1 [HTTP://members.aol.com/rmcdjcamp/dxlabels.htm](http://members.aol.com/rmcdjcamp/dxlabels.htm)
- 2 [HTTP://members.aol.com/rmcdjcamp/defines.htm](http://members.aol.com/rmcdjcamp/defines.htm)

IRUG Spectrum Submission Form

The information requested for submissions is listed below. Terms are defined on the **Numerical Key** on the next page. The **Submission Form** is also available on the **IRUG web site: www.irug.org**. If possible, provide the information in digital format.

IRUG File Name (0): (8 characters assigned by IRUG editors)

Institution (1):

Institution acronym (2):

Address (3):

Analyst (4):

Telephone (5):

Fax (6):

E-mail (7):

Data Description

Institution file name (8) and date/time of acquisition (9):

Format (10):

Sample Description

Common/trade name (11):

Chemical name (12):

Material class (13):

Physical state (14):

Form (15):

Colour/color (16):

Age (17):

Origin

Material source (18):

Source location (19):

Sample identifier (20):

Instrument Parameters

Instrument + software (21):

Spectral range (22):

Resolution (23):

Scans (24):

Apodization (25):

Instrument purge (26): (purge: Y/N)

Technique

Mode (27): (tran/refl/scat)

Accessory (28):

Sample support (29):

Sample preparation (30):

Data Processing History

CO₂ correction (31): (CO₂: Y/N)

Baseline Correction (32): (baseline corr.: Y/N)

Other data processing (33)

Supplemental Analytical Data

Other analytical methods (34):

Additional Information (44 – 57):

Raman Specific Data

Monochromator (35)

Source (36)

Power (37)

Detector (38)

Detector parameters (39)

Collecting lens (40)

Angle (41)

Polarisation (42)

Filters (43)

Numerical Key

- 0 IRUG filename: 8 character filename, beginning "I" for infrared or "R" for Raman, followed by 2 letter IRUG materials class acronym, and a five digit No. assigned and inserted by IRUG editing committee after receipt of the file, e.g., filename: inr00603.dx.
- 1 Originating institution name: full name
- 2 Originating institution acronym: see institution acronym list
- 3 Address: full address of institution
- 4 Analyst: name of analyst who acquired the spectrum
- 5 Telephone: contact telephone # of analyst +/- analytical lab +/- conservation dept., etc
- 6 Fax: contact fax # of analyst +/- analytical lab +/- conservation dept., etc
- 7 Email: contact fax # of analyst +/- analytical lab +/- conservation dept., etc
- 8 Institution filename: 8-character name for spectral file as assigned in originating institution
- 9 Date/time of acquisition: date + time spectrum was acquired
- 10 Format: JCAMP + version number
- 11 Common/trade name: e.g. gypsum, Paraloid B-72
- 12 Chemical name: e.g. calcium sulfate dihydrate, poly(methyl acrylate-ethyl methacrylate) copolymer
- 13 Material Class: **organic**: carbohydrate-gum/sugar (CB), organic pigments and dyes (OD), natural resin (NR), oil/fat (OF), protein (PR), synthetic resin (SR), wax (WX); **inorganic**: minerals, pigments, and corrosion product (MP), glass (GL); **other**: mixtures (MX), unclassified (UC)
- 14 Physical state: solid (s), liquid (l), gas (g)
- 15 Form: chunk, emulsion, flake, fibre/fiber, paste, powder, sheet, etc
- 16 Color /colour: colour of sample material
- 17 Age: approximate age of material, aging history, if known
- 18 Material source: (of sample) manufacturer, supplier, collector, etc
- 19 Source location: country, region, state, city/town, site
- 20 Sample identifier: catalog/catalogue #, CI #, collection #, or any other unique institutional #, e.g. Forbes pigment #, Sigma catalogue/catalog #, etc
- 21 Instrument + software: manufacturer, model, software version
- 22 Spectral range: e.g. 4000 - 650 cm^{-1}
- 23 Resolution: (of spectrum as measured, not of JCAMP file) 4 or 8 cm^{-1} minimum recommended
- 24 Scans: number of scans
- 25 Apodization: boxcar (B), Happ-Genzel (HG), Norton-Beer -weak, medium, strong (NB-w, m, s), triangular (T), etc.
- 26 Instrument purge: Y or N
- 27 Mode: transmission (tran), reflectance (refl), scatter (scat – for Raman)
- 28 Accessory (ies): attenuated total reflectance (atr), beam condenser (bc), diffuse reflectance (drift), fibreoptic (fo), grazing angle (ga), microscope (micr), spectral reflectance (sr), etc
- 29 Sample support(s): AgCl, AgBr, BaF₂, CaF₂, CdTe, CsI, diamond, Ge, KBr, KRS5, NaCl, Nujol (nj), Si, SiC, ZnS, ZnSe, etc
- 30 Sample preparation: neat, CH₂Cl₂ extract, sample ground with KBr, sample and KBr ground separately and mixed, etc
- 31 CO₂ correction: Y or N
- 32 Baseline correction: Y or N
- 33 Other data processing details: spectral subtraction, transformations etc.
- 34 Analytical methods, other (cross-reference): VLM, FLM, PLM, SEM, EDS, EPMA, XRF, AA, ICP, ICP-MS, GC, GC-MS, GC-IR, FT-Raman, RP-HPLC, PAGE, TLC, etc
- 44- Additional information: pathlength, cm (44), pressure (45), temperature °C (46), CAS name (47), molecular formula (48), CAS reg. No (49), Wiswesser line notation (50), Beilstein Lawson No (51), melting point, °C (52), boiling point, °C (53), refractive index (at 20°C for NaD) (54), density g/cm^3 (55), molecular weight (56), concentration (57), etc
- Raman Specific Data:**
- 35 Monochromator: dispersive or interferometric
- 36 Source: excitation source wavelength in nm
- 37 Power: power incident on sample, in mW
- 38 Detector: detector type; CCD, PMT, PDA, etc.
- 39 Detector parameters: integration time, number of accumulations
- 40 Collecting lens: magnification (eg 100x), numerical aperture
- 41 Angle: collecting angle of scattered radiation, in degrees
- 42 Polarisation: polarisation of excitation radiation
- 43 Filters: details of any Notch or interference filters, analyser, etc

IRUG Guidelines for JCAMP-DX Files

(Superscripts ^{1,2...} refer to location of information on **IRUG Sample Submission Form and Numerical Key**)

A	B	C
Labels	IRUG Definition of entries	JCAMP Definition of entries
##TITLE=	<i>insert:</i> IRUG filename ⁰ Common name ¹¹ , material source ¹⁸ , sample identifier ²⁰ , institution acronym ² , mode ²⁷	##TITLE= should contain a concise description of the contents, suitable as a title for a data plot. ##TITLE= is required as the first LDR of each JCAMP-DX FILE or BLOCK.
##JCAMP-DX=	JCAMP version ¹⁰ (4.24)	Required immediately after each ##TITLE= to show Version number of JCAMP-DX. Version of software which generates a JCAMP-DX file should be added as a comment after the Version Number.
##DATA TYPE=	INFRARED SPECTRUM or RAMAN SPECTRUM	##DATA TYPE= defines the data technique for the current JCAMP-DX BLOCK.
Submitting Institution Details		
##ORIGIN=	<i>insert:</i> originating institution name ¹ ; address ³ ; analyst's name ⁴ ; telephone ⁵ ; fax ⁶ ; e-mail ⁷ NB use abbreviations (Tel:, Fax:, Email:) and leave missing data sections blank (e.g.: ... Victoria & Albert Museum, London SW7 2RL, Tel:; Fax: +44 (0)207...)	Name of organization, address, telephone number, FAX number, E-mail address, name of individual contributor, etc., as appropriate. This information is not optional; the originator of a JCAMP-DX file should always see that it is included. The instrument manufacturer cannot be responsible for this information. NOTE: Omission of this information is not necessarily a valid reason for software to refuse to process a JCAMP-DX file. Under no circumstances should a file be retransmitted without this information.
##OWNER=	<i>insert:</i> originating institution name ¹ OR COPYRIGHT © (year) by originating institution name ¹ . (Copyright statement is optional)	Name of owner of proprietary data. The organization or person named under ##ORIGIN= is responsible for accuracy of this field. If the data are copyrighted, this line should read "COPYRIGHT © (year) by (name)." This information is not optional; the originator of a JCAMP-DX file should always see that it is included. If ##OWNER= contains "PUBLIC DOMAIN", the implication is that the data may be copied without permission on the authority of whoever is names under ##ORIGIN=. Absence of ##OWNER= does not imply permission to copy.
##\$License=	<i>insert:</i> By accepting this database user agrees to be bound by the terms of the IRUG user's license. Any reference written/oral made to this file must include accreditation to BOTH the originating individual/institution and IRUG. Contributor agrees to be bound by the terms of the IRUG contributor's license.	IRUG defined data label - no JCAMP definition.

A	B	C
Labels	IRUG Definition of entries	JCAMP Definition of entries
##\$Institution File Name=	<i>insert:</i> originating institution's file name ⁸	IRUG defined data label – no JCAMP definition.
##DATE=	YY/MM/DD date of spectrum acquisition ⁹	Date when data was measured, in the form: YY/MM/DD (note order).
##TIME=	HR/MIN/SEC time of spectrum acquisition ⁹	Time when data was measured, in the form: HR/MIN/SEC (24-hour clock).
Instrument Details		
##SPECTROMETER/ DATA SYSTEM=	<i>insert:</i> instrument and software ²¹ For Raman, <i>include:</i> monochromator ³⁵ ; detector ³⁸	This field contains manufacturer's name, model of the instrument, software system, and release number, as appropriate, in the form used by the manufacturer.
##INSTRUMENT PARAMETERS=	<i>Insert:</i> apodization ²⁵ ; No of scans ²⁴ ; instrument purge ²⁶ ; spectral range ²² For Raman, <i>include:</i> source ³⁶ ; power ³⁷ ; detector parameters ³⁹	This optional field is a list of pertinent instrument settings using standard notation when available, otherwise using the notation of the manufacturer. Only settings which are essential for applications should be included.
##RESOLUTION=	<i>insert:</i> resolution ²³ - of acquired spectrum (not of data in DX file)	Nominal resolution in units specified by ##XUNITS=, as a single number for spectra at constant resolution throughout, or as pairs of the form :R1,X1,...,Rn,Xn, where R stands for Resolution at abscissa X.
##DATA PROCESSING=	<i>insert:</i> entries for CO2 correction ³¹ ; baseline correction ³² ; and any other data processing performed ³³	Description of background correction, smoothing, subtraction, deconvolution procedures, apodization function, zero-fill, or other data processing, together with reference to original spectra used for subtractions.
Sampling Details		
##SAMPLE DESCRIPTION=	<i>insert:</i> mode ²⁷ ; accessory ²⁸ ; sample support ²⁹ For Raman, <i>include:</i> collecting lens ⁴⁰ ; angel ⁴¹ ; polarisation ⁴² ; filters ⁴³	First entry in this field should be MODE of observation (transmission, specular reflection, PAS, matrix isolation, etc., for spectra, or column type, etc., for chromatograms, or ionization parameters, etc. for mass spectra, or appropriate information for any other techniques or applications. Name and model of appropriate accessories, cell thickness, and window material for fixed liquid cells, ATR plate material, angle and cone of incidence, and effective number of reflections for ATR measurements, polarization, and special modulation techniques, as discussed by Grasselli, Griffiths, and Hannah, Appl.Spectroscopy, 1982, 36, 87, etc., are appropriate for other types of measurement. (For V5.0, this information should be under ##APPLICATION=.)
##SAMPLING PROCEDURE=	<i>insert:</i> mode ²⁷ ; and sample preparation ³⁰	First entry in this field should be MODE of observation (transmission, specular reflection). Use enough space to describe the procedure. Give a citation to a description of a standard procedure.
##PATH LENGTH=	<i>insert:</i> pathlength ⁴⁴ , where applicable	Path length in cm.
##PRESSURE=	<i>insert:</i> pressure ⁴⁵ , where significantly different from atmospheric	Sample pressure in appropriate units if significantly different from atmospheric.

A	B	C
Labels	IRUG Definition of entries	JCAMP Definition of entries
##TEMPERATURE=	<i>insert: temperature</i> ⁴⁶ , where significantly different from room temperature	Sample temperature in degrees C if significantly different from room temperature.
Sample Details		
##CAS NAME=	<i>insert: CAS name</i> ⁴⁷ , where available	Name according to Chemical Abstracts naming conventions as described in Appendix IV of the 1985 CAS Index Guide. 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. Sup/Superscripts are indicated by prefixes / and ^, respectively. Example, alpha-D-glucopyranose, 1-(dihydrogen phosphate).
##NAMES=	<i>insert: common/trade name</i> ¹¹ , chemical name ¹² etc. Multiple names placed on separate lines	Common, trade, or other names. Multiple names are placed on separate lines.
##MOLFORM=	<i>insert: molecular formula</i> ⁴⁸ , where available	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 capitalised. The second letter, if required, is in lower case. One-letter symbols must be separated from adjacent symbols by a blank or digit. Sub/super scripts are terminated by the next non-digit. Slash may be omitted for subscripts. For readability, each atomic symbol may be separated from its predecessor by a space. For substances which 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, respectively. Examples: C2H4O2 or C2 H4 O2 (Acetic acid) C6 H9 Cr O6 * H2 O (Chromic acetate monohydrate) H2^17O (water, mass 17 oxygen)
##CAS REGISTRY No=	<i>insert: CAS registry number</i> ⁴⁹ , where available	CAS Registry Numbers for many compounds can be found in Chemical Abstracts indices, Merck Index, or CAS ON-LINE.
##WISWESSER=	<i>insert: Wiswesser line notation</i> ⁵⁰ , where available	The Wiswesser line notation is a precise and concise means of expressing structural formulas as character strings. The basic idea is to use letter symbols to denote functional groups and numbers to express the lengths of chains and the sizes of rings. Wiswesser notation is described in detail by Smith, "The Wiswesser-Line Formula Chemical Notation", McGraw-Hill, New York, 1968), 2nd Ed; and Chemical Information Management, Inc., 3rd Ed, 1975.

A	B	C
Labels	IRUG Definition of entries	JCAMP Definition of entries
##BEILSTEIN LAWSON No=	<i>insert:</i> Beilstein Lawson Number ⁵¹ , where available	The Beilstein Lawson Number is a structural formula clustering code based on the Beilstein System. It is used for locating information in Beilstein databases, including the STN on-line database. The code contains only structural information and can be generated locally on microcomputers from connection table data alone. A simple description of the algorithm has been published by Lawson, "Structure Graphics" in <i>Pointers to Beilstein Out</i> , ACS Symposium 341, Graphics for Chemical Structures - Integration of Text and Data, 1987, pp 80-87.
##MP=	<i>insert:</i> melting point ⁵² , where available	Melting Point in degrees C.
##BP=	<i>insert:</i> boiling point ⁵³ , where available	Boiling Point in degrees C followed by pressure in mm Hg if other than one atmosphere.
##REFRACTIVE INDEX=	<i>insert:</i> refractive index ⁵⁴ , where available	In the form: ND = 1542 ²⁰ (index at 20 degrees C for NaD line).
##DENSITY=	<i>insert:</i> density ⁵⁵ , where available	Density in g/cc.
##MW=	<i>insert:</i> molecular weight ⁵⁶ , where available	Molecular weight.
##CONCENTRATIONS=	<i>insert:</i> concentration ⁵⁷ , where available. Include known impurities	List of known components and impurities and their concentrations in the following form, where N stands for name (enclosed in angle brackets if more than one word); C, for concentration; and U, for units of concentration: EXAMPLE: ##CONCENTRATIONS= (NCU) (N1, C1, U1), (N2, C2, U2), etc. The group for each component is enclosed in parentheses. Each group starts a new line and may continue on the following lines.
##STATE=	<i>insert:</i> physical state ¹⁴ and form ¹⁵ (For IRUG, sample prep is under ##Sampling Procedure)	Solid, liquid, gas, solution, KBr pellet, powder, nujol mull, etc.
##CROSS REFERENCE=	<i>insert:</i> all supplemental/other analytical methods ³⁴	Cross references refer to additional data on the same sample, i.e., different thickness, mulling agent, polarisation, temperature, time, etc., or serve to link a peak table or interferogram with a spectrum, etc.
Additional IRUG sample details		
##\$Material Source	<i>insert:</i> material source ¹⁸	IRUG defined data label – no JCAMP definition.
##\$Source location	<i>insert:</i> source location ¹⁹	IRUG defined data label – no JCAMP definition.
##\$Sample Identifier	<i>insert:</i> sample identifier ²⁰	IRUG defined data label – no JCAMP definition.
##\$Colour=	<i>insert:</i> color/colour ¹⁶	IRUG defined data label – no JCAMP definition.

A	B	C
Labels	IRUG Definition of entries	JCAMP Definition of entries
##\$Age=	<i>insert: age</i> ¹⁷	IRUG defined data label – no JCAMP definition.
##\$IRUG Material Class=	<i>insert: materials class</i> ¹³	IRUG defined data label - no JCAMP definition.
##=	<i>insert: any additional information</i>	Comments may be introduced by a DATA-LABEL-FLAG (##) plus a DATA-LABEL-TERMINATOR (=), with null DATA-LABEL-NAME. Such comments may continue for more than one line, terminating at the next DATA-LABEL-FLAG. Sub-headings (not JCAMP-DX Labels) may be used within such comments at the discretion of the end-user. As many such comments as needed may be included between ##TITLE= and ##END=.
Spectral Information		
##DELTA=	Automatically inserted by commercial software converter	This LDR gives the nominal spacing between points for informing the user. Actual X-values should be calculated from (##LASTX= minus ##FIRSTX=)/(##NPOINTS= - 1).
##XUNITS=	Automatically inserted by commercial software converter, 1/cm preferred	##XUNITS= gives the abscissa units for the current DATA TYPE. Any standard unit is acceptable. For infrared spectra, the following units are appropriate: 1/CM (representing wavenumber), MICROMETERS, NANOMETERS, SECONDS, ARBITRARY UNITS
##YUNITS=	Automatically inserted by commercial software converter: absorbance / transmittance /arbitrary units... For maximum compatibility, IR spectra for submission to IRUG should be in ABSORBANCE. For Raman, this should be RELATIVE INTENSITY .	Gives the ordinate units for the current DATA TYPE. Any standard units are acceptable. For infrared spectra, the following units are appropriate: TRANSMITTANCE, REFLECTANCE, ABSORBANCE, KUBELKA-MONK, ARBITRARY UNITS
##XFACTOR=	Automatically inserted by commercial software converter	##XFACTOR= and ##YFACTOR= ,respectively, are factors by which components of tabulated abscissa and ordinate values should be multiplied to obtain actual values. For ASCII representation, these factors should be chosen to convert tabulated values to integers, clipping off all but about 1 digit of noise on the average.
##YFACTOR=	Automatically inserted by commercial software converter	
##FIRSTX=	Automatically inserted by commercial software converter	##FIRSTX= and ##LASTX= are the first and last ACTUAL abscissa values for current DATA TYPE, as appropriate. First tabulated abscissa time ##XFACTOR= should equal ##FIRSTX=.
##LASTX=	Automatically inserted by commercial software converter	Spectral data are tabulated in order of EITHER increasing or decreasing abscissa values. ##FIRSTX= specifies the abscissa corresponding to the first value listed under the current DATA TYPE, not the smallest abscissa.
##NPOINTS=	Automatically inserted by commercial software converter	##NPOINTS= is the number of components of a ##DATACLASS= like ##XYDATA=.

A	B	C
Labels	IRUG Definition of entries	JCAMP Definition of entries
##FIRSTY=	Automatically inserted by commercial software converter	##FIRSTY= is the actual Y-value corresponding to ##FIRSTX=. ##FIRSTY= should equal ##YFACTOR= times the first Y-value in the current ##DATACLASS=. NOTE: If the ordinate value corresponding to ##FIRSTX= is undefined, i.e., represented by ?, then ##FIRSTY= also is represented by ?. This is the reason for recommending the different way of checking data scaling which is outlined under ##MAXX=, etc.
##MAXY= ##MAXX=	Automatically inserted by commercial software converter	These attributes of the data array were listed as OPTIONAL in V4.24. It is currently recommended that ##MAXY= and ##MINY= be required for ##XYDATA=. It is now recommended that the difference ##MAXY= minus ##MINY= be compared to the difference between converted values to check Ordinate scaling rather than comparing ##FIRSTY= to the product of ##YFACTOR= and the first converted ordinate as recommended in V4.24. See NOTE under ##FIRSTY=
##MINY= ##MINX=	Automatically inserted by commercial software converter	
##XYDATA=	Automatically inserted by commercial software converter	##XYDATA= is the heading for a data array which consists of a list or ordinates at equal X-intervals, as specified by the following Data Labels: ##XUNITS=, ##YUNITS=, ##XFACTOR=, ##YFACTOR=, ##FIRSTX=, ##LASTX=, ##MAXY=, ##MINY=, ##NPOINTS=, ##FIRSTY=. The tabular form of the ##XYDATA= is a series of lines organized as follows: X1 Y1 Y2 Y3 Y4 Y5 ... YN. This form of data is represented symbolically by a VARIABLE LIST, as follows: ##XYDATA= (X++(Y..Y)), - where X++ indicates that the first item in a line is an X-value, ++ indicates that X is incremented for each following Y-value and (Y..Y) indicates that the initial X-value is followed by a succession of Y-values
...	Automatically inserted by commercial software converter, data...	
##End=		##END= indicates the end of a JCAMP-DX FILE or BLOCK. There must be one ##END= for each ##TITLE= in a COMPOUND JCAMP-DX file.

General Format for IRUG Infrared JCAMP-DX Files

(Numbers in brackets refer to location of the information on the IRUG Sample Submission Form and Numerical Key)

##TITLE=[IRUG filename (0)] [Common/trade name (11)], [sample source (19)], [sample identifier (20)],
[INSTITUTION ACRONYM (2)], [mode (27)]
##JCAMP-DX=4.24
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=[originating institution (1)]; [address (3)]; [analyst (4)]; tel: [telephone (5)]; fax: [fax (6)]; email: [e-mail (7)]
##OWNER=COPYRIGHT © [year] by [institution name (1) or acronym (2)]
##\$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. Any reference written/oral made to this file must
include accreditation to BOTH the originating individual/institution and IRUG.
Contributor agrees to be bound by the terms of the IRUG contributor's license.
##\$INSTITUTION FILE NAME=[institution filename (8)]
##DATE=[date/time of acquisition (9)]
##TIME=[date/time of acquisition (9)]
##SPECTROMETER/DATA SYSTEM=[instrument and software (21)]
##INSTRUMENT PARAMETERS= apodization: [apodization (25)]; scans: [No of scans (24)]; purge: [instrument
purge Y/N (26)]; range: [spectral range (22)]
##RESOLUTION=[resolution (23)]
##DATA PROCESSING= CO2 corr.: [CO2 correction Y/N (31)]; baseline corr.: [baseline correction Y/N (32)]; [other
data processing (33)]; further data processing information may automatically be inserted by JCAMP converter
##SAMPLE DESCRIPTION= [mode (27)]; accessories: [accessory (28)]; support: [sample support (29)]
##SAMPLING PROCEDURE=[mode (27)]; prep: [sample preparation (30)]
##PATHLENGTH=[pathlength (44)]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES=[common/trade name (11)]
[chemical name (12)]
##MOLFORM=[molecular formula (48)]
##CAS REGISTRY NUMBER=[CAS registry number (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson number (51)]
##MP=[melting point (52)]
##BP=[boiling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentrations (57)]
##STATE=[physical state (14)]; [form (15)]
##CROSS REFERENCE=[other analytical methods (34)]
##\$MATERIAL SOURCE=[source of sample(18)]
##\$SOURCE LOCATION=[source location (19)]
##\$SAMPLE IDENTIFIER=[sample identifier (20)]
##\$COLOUR=[color/colour (16)]
##\$AGE=[age (17)]
##\$IRUG MATERIALS CLASS=[material class (13)]
##DELTA=[automatically inserted]
##XUNITS=[automatically inserted]
##YUNITS=[automatically inserted]
##FIRSTX=[automatically inserted]
##LASTX=[automatically inserted]
##FIRSTY=[automatically inserted]
##MAXX=[automatically inserted]
##MINX=[automatically inserted]
##MAXY=[automatically inserted]
##MINY=[automatically inserted]
##XFACTOR=[automatically inserted]
##YFACTOR=[automatically inserted]
##NPOINTS=[automatically inserted]
##XYDATA=[automatically inserted] 624.823
##END=[automatically inserted]

General Format for IRUG Raman JCAMP-DX Files

(Numbers in brackets refer to location of the information on the IRUG Sample Submission Form and Numerical Key)

```
##TITLE=[IRUG filename (0)] [Common/trade name (11)], [sample source (19)], [sample identifier (20)],
[INSTITUTION ACRONYM (2)], scat (27)
##JCAMP-DX=4.24
##DATA TYPE=RAMAN SPECTRUM
##ORIGIN=[originating institution (1)]; [address (3)]; [analyst (4)]; tel: [telephone (5)]; fax: [fax (6)]; email: [e-mail (7)]
##OWNER=COPYRIGHT © [year] by [institution name (1) or acronym (2)]
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. Any reference written/oral made to this file must
include accreditation to BOTH the originating individual/institution and IRUG.
Contributor agrees to be bound by the terms of the IRUG contributor's license.
##$INSTITUTION FILE NAME=[institution filename (8)]
##DATE=[date/time of acquisition (9)]
##TIME=[date/time of acquisition (9)]
##SPECTROMETER/DATA SYSTEM=[instrument and software (21)]; monochromator: [dispersive / interferometric
monochromator (35)]; detector: [detector type (38)]
##INSTRUMENT PARAMETERS= apodization: [apodization (25)]; scans: [No of scans (24)]; purge: [instrument
purge Y/N (26)]; range: [spectral range (22)]; source: [source (36)]; power: [power (37)]; detector parameters:
[detector parameters (39)]
##RESOLUTION=[resolution (23)]
##DATA PROCESSING= CO2 corr.: [CO2 correction Y/N (31)]; baseline corr.: [baseline correction Y/N (32)]; [other
data processing (33)]; further data processing information may automatically be inserted by JCAMP converter
##SAMPLE DESCRIPTION= scat; accessories: [accessory (28)]; support: [sample support (29)]; objective: [collecting
lens (40)]; angle: [angle (41)]; polarisation: [polarisation (42)]; filters: [filters (43)]
##SAMPLING PROCEDURE=scat; prep: [sample preparation (30)]
##PATHLENGTH=[pathlength (44)]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES=[common/trade name (11)]
[chemical name (12)]
##MOLFORM=[molecular formula (48)]
##CAS REGISTRY NUMBER=[CAS registry number (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson number (51)]
##MP=[melting point (52)]
##BP=[boiling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentrations (57)]
##STATE=[physical state (14)]; [form (15)]
##CROSS REFERENCE=[other analytical methods (34)]
##$MATERIAL SOURCE=[source of sample(18)]
##$SOURCE LOCATION=[source location (19)]
##$SAMPLE IDENTIFIER=[sample identifier (20)]
##$COLOUR=[color/colour (16)]
##$AGE=[age (17)]
##$IRUG MATERIALS CLASS=[material class (13)]
##DELTA=[automatically inserted]
##XUNITS=[automatically inserted]
##YUNITS=Relative intensity
##FIRSTX=[automatically inserted]
##LASTX=[automatically inserted]
##FIRSTY=[automatically inserted]
...
...
##XFACTOR=[automatically inserted]
##YFACTOR=[automatically inserted]
##NPOINTS=[automatically inserted]
##XYDATA=[automatically inserted] 624.823 .....
##END=[automatically inserted]
```

Institution Acronym Key for Database Contributors as of July 2000

ADSL	Archaeological Department, Colombo, Sri Lanka, LK
AFA-V	Academy of Fine Arts, Institute of Chemistry, Vienna, AU
AIC	Art Institute of Chicago, Chicago, IL, US
AMNH	American Museum of Natural History, New York, NY, US
BM	British Museum, London, GB
BSU	Ball State University, Muncie, IN, US
CCI	Canadian Conservation Institute, Ottawa, CA
CIA	Courtauld Institute of Art, University of London, GB
COA-CNR	Centro Opere D'Arte, Consiglio Nazionale delle Ricerche, Firenze, IT
CU	Cardiff University, School of History and Archaeology, Cardiff, Wales, GB
deYNG	M.H. De Young Museum, San Francisco, CA, US
FAUK	Department of Fine Arts, University of Kelaniya, Kelaniya, Sri Lanka, LK
FGA	Freer Gallery of Art, Smithsonian Institution, Washington, DC, US
FU	CECOR – Escola de Bela Artes, Federal University of Minas Gerais, BR
GACC	Garbar Art Conservation Center (Russian Scientific Conservation Center named after Grabar), Moscow, RU
GCI	Getty Conservation Institute, Los Angeles, CA, US
HKI	Hamilton Kerr Institute, Cambridge, GB
HNM	Hungarian National Museum, Budapest, HU
IROE-CNR	Istituto di Ricerca Sulle Onde Elettromagnetiche, Consiglio Nazionale delle Ricerche, Firenze, IT
LMU	Loyola Marymount University, Los Angeles, CA, US
MASCA	Museum Applied Science Center for Archaeology, University of Pennsylvania, Philadelphia, PA, US
McC	McCrone Research Institute, Chicago, IL, US
MFA-B	Museum of Fine Arts Boston, Boston, MA, US
MMA	Metropolitan Museum of Art, New York, NY, US
MNRS	Museo Nacional Reina Sofia, Madrid, ES
MOMA	Museum of Modern Art, New York, NY, US
MU	Miami University, Oxford, OH, US
NARA	National Archives and Records Administration, Washington, DC, US
NG	National Gallery, London, GB

NGA	National Gallery of Art, Washington, DC, US
NMGM	National Museums and Galleries on Merseyside, Liverpool, GB
NMWA	National Museum of Western Art, Tokyo, JP
NSC	National School of Conservation, Mexico City, MX
OADC	Ormylia Art Diagnosis Centre, Ormylia, GR
PMA	Philadelphia Museum of Art, Philadelphia, PA, US
RFL	Rathgen –Forschungslabor, Staatliche Museen Preußischer Kulturbesitz, Berlin, DE
SC	School of Conservation, Det Kongelige Danske Kunstakademi, Copenhagen, DK
SCC	Straus Conservation Center (Fogg), Harvard University Art Museums, Cambridge, MA, US
TG	Tate Gallery, London, GB
UF	University of Florence, Firenze, IT
UI	University of Iceland, Reykjavik, IS
UM	Micro-analytical Research Centre, School of Physics, University of Melbourne, VIC 3010, AU
VA	Victoria and Albert Museum, London, GB
WACC	Williamstown Art Conservation Center, Williamstown MA, US
WM	Winterthur Museum, Garden and Library, Winterthur, DE, US

Example 1A

JCAMP-DX file as generated by Nicolet converter.

```
##TITLE=PMAI2037 SEEDLAC NO. 4858 AF SUTER & CO LTD
##JCAMP-DX=4.24 $$ Nicolet v. 410
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=PMA Conservation Dept.
##OWNER=Nicolet
##DATE=98/06/30
##TIME=13:45:06
##DATA PROCESSING=
Ratio against background
%Transmittance->Absorbance
Straight Line generate
Truncated
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=624.823181
##LASTX=3999.639893
##FIRSTY=0.029192
##MAXX=3999.639893
##MINX=624.823181
##MAXY=0.981087
##MINY=-0.001622
##XFACTOR=1.000000
##YFACTOR=1.000000E-009
##NPOINTS=1751
##DELTA X=1.928467
##XYDATA=(X++(Y..Y))
624.823 ...
...
##END=
```

Example 1B

Same JCAMP-DX file edited to meet IRUG guidelines.

```
##TITLE=INR00610 Seedlac, AF Suter, #4858, PMA, tran
##JCAMP-DX=4.24 $$ Nicolet v. 410
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=Philadelphia Museum of Art; Box 7646, Philadelphia, PA 19101, USA; Beth
Price; tel:+1 215 684 7552; fax: +1 215 684 7550; email: bprice@philamuseum.org
##OWNER=COPYRIGHT © 98 by Philadelphia Museum of Art, Cons Dept Analytical Lab
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. ...
##$INSTITUTION FILE NAME=PMAI2037
##DATE=98/06/30
##TIME=13:45:06
##SPECTROMETER/DATA SYSTEM=Nicolet 510P bench w/ NIC-Plan micr; OMNIC v2.1
##INSTRUMENT PARAMETERS=apodization: HG; scans: 200; purge: dry air; range: 4000
-625 cm-1
##RESOLUTION=4 cm-1
##DATA PROCESSING=CO2 corr.:Y; baseline corr.:Y; Multiplied by a scalar,
Converted from OMNIC, Ratio against background, Straight Line gen., Truncated
##SAMPLE DESCRIPTION=tran; accessories: micr; support: dia
##SAMPLING PROCEDURE=tran; prep: scraping
##PATHLENGTH=[pathlength (44)]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES=seedlac
[chemical name (12)]
##MOLFORM=[molecular formula (48)]
##CAS REGISTRY NUMBER=[CAS registry No (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson No (51)]
##MP=[melting pont (52)]
##BP=[boiling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentration (57)]
##STATE=solid; bulk
##CROSS REFERENCE=GC-MS
##$MATERIAL SOURCE=AF Suter & Co, Ltd
##$SOURCE LOCATION=London, England, UK
##$SAMPLE IDENTIFIER=AF Suter #4858
##$COLOR=orange-brown
##$AGE=unknown, purchased 1996
##$IRUG MATERIALS CLASS=NR
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=624.823181
##LASTX=3999.639893
...
##XYDATA=(X++(Y..Y))
624.823 .....
##END=
```

Example 2A

JCAMP-DX file as generated by Perkin-Elmer converter.

```
##TITLE= Cellulose nitrate by SiC. Millipore SC 8micron. GLM
##JCAMP-DX= 4.24
##DATA TYPE= INFRARED SPECTRUM
##ORIGIN= Exported PE Spectrum Data File
##OWNER=
##DATE= 94/05/04
##TIME= 14:31:19.00
##SPECTROMETER/DATA SYSTEM= PERKIN-ELMER Not Specified IR
##INSTRUMENT PARAMETERS=
  APODIZATION=Not Specified
  DETECTOR=Not Specified
##RESOLUTION= 1.000000
##DELTAX= -1.000000
##XUNITS= 1/CM
##YUNITS= TRANSMITTANCE
##XFACTOR= 1.00
##YFACTOR= 0.00000023841857910156
##FIRSTX= 4000.00
##LASTX= 400.00
##NPOINTS= 3601
##FIRSTY= 55.46
##MAXY= 9.209990
##MINY= 163.83
##XYDATA= (X++(Y..Y))
4000.000000 687173699 687173699 ...
...
##END=
```

Example 2B

Same JCAMP-DX file edited to meet IRUG guidelines.

```
##TITLE=ISR05000 Cellulose nitrate, VA, refl
##JCAMP-DX= 4.24
##DATA TYPE= INFRARED SPECTRUM
##ORIGIN= Victoria & Albert Museum; South Kensington; GB London SW7 2RL; Boris
Pretzel; tel:+44 (0)20 7942 2116; fax:+44 (0)20 942 2092; email:
boris.pretzel@vam.ac.uk
##OWNER=COPYRIGHT © 1989 by Victoria & Albert Museum
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. Any reference...
##$INSTITUTION FILE NAME=DR0008
##DATE=89/05/04
##TIME=13:45:06
##SPECTROMETER/DATA SYSTEM= PERKIN-ELMER 1730
##INSTRUMENT PARAMETERS=apodization: NB(weak); scans: 250; purge: N;
range: 4000-400
##RESOLUTION=8 cm-1
##DATA PROCESSING=CO2 corr.: N; baseline corr: N
##SAMPLE DESCRIPTION= refl; accessories: drift, Barnes Diffuse Reflectance;
support: SiC
##SAMPLING PROCEDURE= refl; prep: surface sampled with Millipore SiC 8 microns.
Direct from SiC, ratioed to blank SiC (background)
##PATHLENGTH=[pathlength (44)]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES= cellulose nitrate
[chemical name (12)]
##MOLFORM=(C6H10O5)x(ONO2)y
##CAS REGISTRY NUMBER=[CAS registry No (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson No (51)]
##MP=[melting pont (52)]
##BP=[boiling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentration (57)]
##STATE=solid; FILM
##CROSS REFERENCE=GC-MS
##$MATERIAL SOURCE=British Museum
##$SOURCE LOCATION=London WC1B 3DG, England, UK
##$SAMPLE IDENTIFIER=
##$COLOUR=transparent
##$AGE=50 years
##$IRUG MATERIALS CLASS=SR
##DELTAX= -1.000000
...
...
##END=
```

Example 3A

JCAMP-DX file as generated by Analect converter.

```
##TITLE=Yellow refined beeswax , Ross Wax Co.
##JCAMP-DX=4.24
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=.Winterthur
##OWNER=Winterthur
##SAMPLING DESCRIPTION=Winterthur Museum Analytical Laboratory
##Spectrometer/Data System=Analect Instruments. Analect DS-20
##RESOLUTION=4.0
##DATE=97/07/09
##TIME=10:18:30
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=4400.762
##LASTX=698.01
##FIRSTY=0.1153
##XFACTOR=1.000000
##YFACTOR=0.000091553
##NPOINTS=2075
##DELTA X=1.92846702
##XYDATA=(X++(Y..Y))
4400.762 1356337920 .....

##END=
```

Example 3B

Same JCAMP-DX file edited to meet IRUG guidelines.

```
##TITLE=IWX05000 Beeswax, refined, yellow, Ross Wax, WM, tran
##JCAMP-DX=4.24
##DATA TYPE=INFRARED SPECTRUM
##ORIGIN=Winterthur Museum; Winterthur, DE 19735. USA; Janice Carlson; tel:
+1 302 888 4732; fax: +1 302 888 4838; email: jcarls@winterthur.org
##OWNER=COPYRIGHT© 97 by Winterthur Museum
##$LICENSE=By accepting this database user agrees to be bound by the terms of
the IRUG user's license. Any reference...
##$INSTITUTION FILE NAME=WMwax1
##DATE=97/0709
##TIME=10:18:30
##SPECTROMETER/DATA SYSTEM=Analect RFX-65 bench with XAD microscope; DS-20
##INSTRUMENT PARAMETERS=apodization: HG; scans: 200; purge: Y dry air;
range: 4400-700
##RESOLUTION=4 cm-1
##DATA PROCESSING=CO2 corr: N; baseline corr: N; converted from Analect
##SAMPLE DESCRIPTION=tran; accessories: micr; support: dia
##SAMPLING PROCEDURE=tran; prep: scraping
##PATHLENGTH=[pathlength (44)]
##PRESSURE=[pressure (45)]
##TEMPERATURE=[temperature (46)]
##CAS NAME=[CAS name (47)]
##NAMES=beeswax, yellow refined
[chemical name (12)]
##MOLFORM=[molecular formula (48)]
##CAS REGISTRY NUMBER=[CAS registry No (49)]
##WISWESSER=[Wiswesser line notation (50)]
##BEILSTEIN LAWSON No=[Beilstein Lawson No (51)]
##MP=[melting pont (52)]
##BP=[boiling point (53)]
##REFRACTIVE INDEX=[refractive index (54)]
##DENSITY=[density (55)]
##MW=[molecular weight (56)]
##CONCENTRATIONS=[concentration (57)]
##STATE=solid; bulk
##CROSS REFERENCE=[additional information (33)]
##$MATERIAL SOURCE=Ross Wax Co.
##$SOURCE LOCATION=New York, USA
##$SAMPLE IDENTIFIER=unknown
##$COLOUR=yellow, pale
##$AGE=unknown
##$IRUG MATERIALS CLASS=WX
##XUNITS=1/CM
##YUNITS=ABSORBANCE
##FIRSTX=4400.762
##LASTX=698.01
...
##END=
```