Proposed International Standard for EMR spectroscopic data

Richard Cammack[1], Yang Fann[2], Robert J. Lancashire[3‡], John P. Maher[4], Peter S. McIntyre[5], and Reef Morse[6]

[1] Pharmaceutical Sciences Research Division, King's College, Franklin-Wilkins Building, 150 Stamford St, London SE1 9NH, U.K.; [2] Science Task Manager, Information Technology Support Services, NIEHS/NIH, P.O. Box 12233, MD F0-02, Research Triangle Park, NC 27709, U.S.A.;
[3] Department of Chemistry, University of the West Indies, Mona, Kingston 7, Jamaica; [4] now retired, School of Chemistry, University of Bristol, Bristol BS8 1TS, United Kingdom;
[5] School of Applied Sciences, University of Glamorgan, Pontypridd, Mid-Glamorgan, CF37 1DL, United Kingdom; [6] Reef Morse, Scientific Software Services, 42583 Five Mile Road, Plymouth, MI 48170, U.S.A.

Oh, No ! I brought the music for a Jeol, but this is a Bruker harpsichord.

Sound familiar ?

JCAMP-DX (named after the Joint Committee on Atomic and Molecular Physical Data Exchange Standards) is a set of standard formats for exchange of spectroscopic and similar data. It is supported by IUPAC and other international scientific unions.

The protocols were developed for the exchange of infrared spectra, and have been extended to chemical structures, nuclear magnetic resonance data, mass spectra and ion mobility spectra, etc. These are supported by all the major instrument manufacturers.

Features

- open-source
- a single file contains a spectrum or block of spectra
- standardized for web display and internet transmission
- archivable in readily readable format (plain ASCII)
- standard non-proprietary protocols for data compression
- terms used are standard within JCAMP-DX format
- accessed by generic software for JCAMP-DX
- straightforward to convert from other formats

Examples of applications

- transmitting spectra over the internet
- displaying them on standard browsers
- archiving of EMR spectra from any source
- linking spectroscopic data to other chemical information

View the latest draft at http://www.jcamp.org

IUPAC
Committee on Printed and Electronic Publications
Subcommittee on Electronic Data Standards (SEDS)

The **International Union of Pure and Applied Chemistry (IUPAC)** has a long history in the development and support of scientific data standards. In 1995 IUPAC took over responsibility for the JCAMP-DX range of scientific standards from the Joint Committee on Atomic and Molecular Physical Data (JCAMP) and a IUPAC Working Party had responsibility for the support and development of the JCAMP-DX scientific data standards.
In 2003, due to the increasing interest in the use of the Extensible Markup Language for data exchange, the Working Party evolved into the Subcommittee for Electronic Data Standards with oversight duties within IUPAC for all activities in either the JCAMP-DX sphere or the XML in Chemistry area.

News & Notices

Sourceforge – check for code to read and write JCAMP-DX data files at http://sourceforge.net/projects/jcamp-dx/

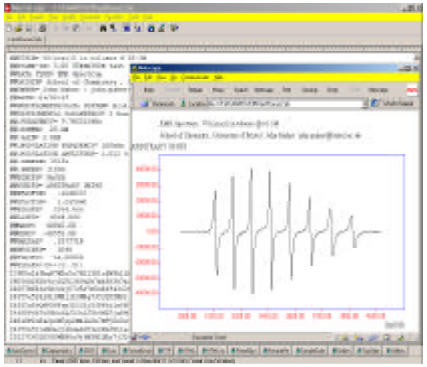
XML in Chemistry - new IUPAC initiative to bring a degree of regulation to this important and rapidly expanding field. (see http://animl.sourceforge.net)

Terms for EMR JCAMP-DX format

Parameter	Allowable words & units	Comments
##TITLE=	TEXT	REQUIRED
##JCAMP-DX=	5.2 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	REQUIRED
##.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, etc.	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 for 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 SIMULATION
##.SIMULATION PARAMETERS	TEXT	REQUIRED FOR SIMULATION
##SAMPLE DESCRIPTION=	TEXT	REQUIRED
##CAS NAME=	TEXT	OPTIONAL
##STATE=	Solid, liquid, gas, etc.	TEXT, OPTIONAL
##CONCENTRATION=	TEXT	OPTIONAL
##XUNITS=	DEGREES, HERTZ, KELVIN, SECONDS, TESLA, WATTS	to be used as XLABEL if ##XLABEL is undefined. STRING, 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
##LASTX=	NUMBER	REQUIRED
##NPOINTS=	POSITIVE INTEGER	REQUIRED
##FIRSTY=	NUMBER	REQUIRED
##$NOTES	TEXT	from legacy data
##END=		REQUIRED

Example of web browser display

(Not all parameters implemented yet)



Comments, please !

IUPAC standards are agreed after consultation with users. So we are asking spectroscopists, programmers and instrument manufacturers to comment on our recommendations.

e-mail to :
Prof. R.J. Lancashire **robert.lancashire@uwimona.edu.jm**

Credits

This project is funded by the International Union of Pure and Applied Chemistry (IUPAC). We thank Bruker and JEOL for their advice in developing this standard.

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