JCAMP-DX to Origin utility Tools for making spectra available to chemometricians

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One of the major uses of the data standards technology we have been pushing over the years is in the communication between analytical instrumentation and data analysis packages. Unfortunately the ability of the more advanced research mathematics packages to "understand" spectroscopy or spectroscopic data formats out-of-the box continues to be disappointing. In the early days of chemometrics research on the problem of non-invasive blood glucose analysis, the needs of the signal processing expert Ralf Marbach clashed with the reality of typical mathematics packages. Although Mike Heise's team were starting to collect some extremely interesting data in the infrared and near infrared spectral regions, the guy who had to carry out the number crunching was stuck with having to enter the numeric data by hand.

The problem was solved by programming import filters for the early JCAMP-DX file format into packages like Mathematica, Matlab etc. The advantages of using an ASCII format were quickly grasped.

In later years the different groups working in ISAS have to a large extent standardised on the use of a package called Origin to carry out data analysis, visualisation and reporting. Here again the need for simple tools to get the spectroscopic data into the analysis software reappeared and were solved in the usual manner.

However, this time there has been one difference. In agreement with the authors and management of the ISAS we are happy to be able to make these latest utilities for reading standard infrared and near infrared JCAMP-DX files available to readers of *Spectroscopy Europe*.

Downloading the utilities

There are two utilities available for downloading on the ISAS web site under the URL:

http://www.ansci.de/downloads/jcamp/

The JCAMP to ASCII executable and the JCAMP DLL itself have been made available with the respective source code. The JCAMP DLL was tested under the Windows 98, NT4, 2000 and XP operating systems. The utilities were tested on Origin 6.0 and 7.0 as well as with Origin Pro versions 6.1, 7.0 and 7.5.

Anyway, having now downloaded the files and read the GNU general public license under which these utilities are being made available you are ready to install the tools.

1. Unpack the ZIP file JcampDLL.zip.
2. Copy the Dynamic Link Library (DLL) "jcamp.dll" either into the Origin installation directory (e.g. C:\Program Files\OriginLab\Origin7G\) or in to a directory that lies in the search path (PATH). If in doubt for your particular installation search for *.OTW in the ORIGIN directory tree and copy the JCAMP.DLL into the uppermost directory where these files are found.
3. The Origin Worksheet Template "JCAMP.OTW" also needs to be copied to the Origin installation directory or to a data directory.

Using the jcamp.dll utility

1. Open the Origin Worksheet Template "JCAMP.OTW".
2. Press the button "JCAMP-DX Import".
3. A window will now open and you can navigate around your environment or network in the usual way until you have found the JCAMP-DX file you wish to import. Highlight this file and

click on "open". If you activate the "Show Info" check box the content of the first line of the JCAMP-DX file (##TITLE= …) will appear in the comment box (Figure 1).
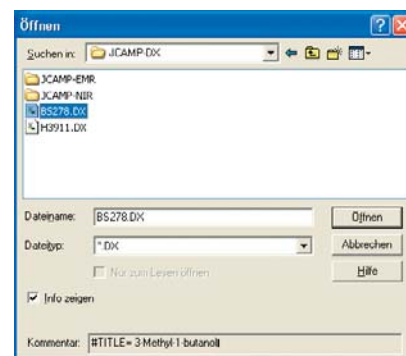

Figure 1.

4. The first column of the worksheet reads in the abscissa values and the second the ordinates. The time which is stored in either the JCAMP-DX LDR ##TIME= or ##LONG DATE=, is imported as a dataset label which can be seen above the Y-column. The name of the JCAMP-DX file is imported as the worksheet name and the title (##TITLE=) as the worksheet label (Figure 2).
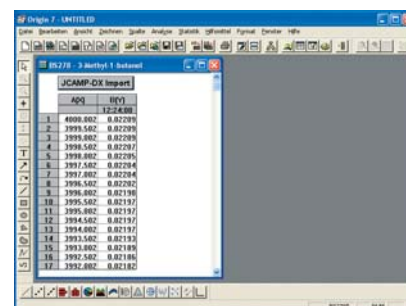

Figure 2.

5. With the data loaded it is now possible to generate plots of the spectra. If the reversed wavenumber display is required for infrared spectra this should be carried out by hand clicking on the x-axis in the plot, right mouse click to open the x-axis options box and select properties where you can alter all of the axis properties including first and last values (Figure 3). Currently the x- and y-axis labels are not read from the JCAMP-DX file and so these must be added by clicking on the labels in the plot and editing by hand.
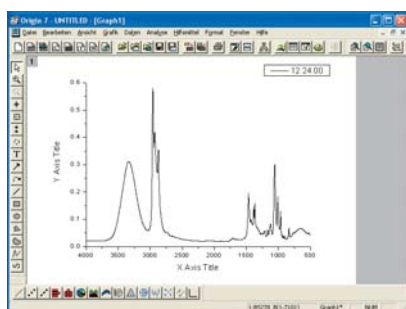
Figure 3.

6. The tools can also handle multiple spectra where they are stored in a compound JCAMP-DX file (not NTUPLES). The x-axis needs to be the same for all of the spectra in the data set, as Origin will take the x-axis of the first file and use this for the rest of the data in the array. The tool then imports only the y-values from the remaining spectra. The utility has been tested up to 500 spectra and 2000 data points per spectrum (1 million y-values) without problem. (Figure 4).
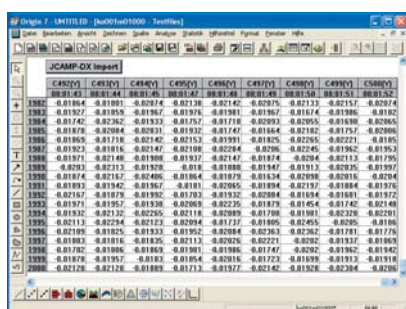

Figure 4.

Restrictions

- Currently the tool only reads data stored using the more complicated ##XYDATA= JCAMP-DX format. The simpler XY pair formats such as ##XYPOINTS=, Peak lists and Peak Assignments are not supported. These is no great problem as the peak lists and assignments can be read into Origin using the ascii import functions.

- Currently data in the ##NTUPLES= format are also not imported as ISAS does not have any instruments generating data using this format. Although a perfectly valid data format option, the more modern ##NTUPLES= option is currently only implemented at ISAS for NMR FIDs. To date such an import of FIDs to Origin has not been requested!

- During testing with older JCAMP-DX files, a further problem arose when LabCalc JCAMP-DX files with real numbers (rather than the usual integers) in the data section were encountered.

Technical background information

The button "JCAMP-DX Import" starts a LabTalk script. This script is stored in the worksheet-template JCAMP.OTW. The script starts by opening a window to allow the user to locate and select the JCAMP-DX file to be imported. The file type *.dx is set as the default but this can be altered to *.jdx or to *.* should this be necessary. Once the JCAMP-DX file has been loaded the worksheet is renamed, taking on the same name as the original JCAMP-DX file without the file extension.

Finally, the JCAMP.DLL is called to parse the JCAMP-DX file. The LabTalk command is:

```
DLL jcamp dx2org %H %B%A;
```

(please note the single space between %H and *%B%A and* no space between %B and %A – important!!)

Here **jcamp** is the name of the DLL being called, **dx2org** the name of function within the DLL, **%H** is a LabTalk system variable which contains the name of the active window and **%B%A** are two more system variables which contain the path and the name of the JCAMP-DX file to be imported. This command line can be integrated into your own LabTalk scripts if desired so long as the system variables are set as described.

Export of JCAMP-DX files to Excel or Matlab

The function **dx2org** is only one of the functions within the JCAMP.DLL. A further export function AsciiExport can be called using:

```
int AsciiExport(const char *InputFile, const char *OutputFile, const char *separator);
```

This function can be used, for example, by C or C++ programs in order to generate ASCII files from JCAMP-DX. An example of such use is provided in the second download where the interface is programmed into the demo program

Dx2Asc.exe. The program is started from a command line (from DOS prompt):

```
C:\> Dx2Asc jcampfile.dx textfile.csv
```

The program creates a text file with the x- and y-values separated by a comma. In this manner a JCAMP-DX file can be converted into a CSV file for direct import into Excel or Matlab. The JCAMP.DLL must be in the current directory or in one of the directories listed under PATH.

Dx2Asc is only a very simple program and aims to demonstrate the function call **AsciiExport()**.

Launching Dx2Asc.exe in Matlab

This command line program has the advantage over Windows applications that it can be integrated into other software systems such as Matlab programs (.m files), e.g.

```
>> error = dos('Dx2Asc.exe jcampfile.dx textfile.csv ','-echo');
```

The Matlab function **dos()** has two parameters, the function call for the external program Dx2Asx.exe as well as the option **–echo**. This option re-directs the output of the external program to the Matlab window. The return value of the external program is stored in the variable **error**. When Dx2Asc.exe terminates with errors then the returned value is 0.

Details of the download

The compiled versions and the source code of the JCAMP.DLL and the demonstration program Dx2Asc.exe are available at the internet address shown above. The software has been written with Borland C++ Builder 5.0. The Borland project files are also in the ZIP files. The software is made available under the GNU GPL Licence. The copyright remains with ISAS in Dortmund.

If anyone else has utilities they would be prepared to release to help us all then please get in touch and we might be able to start a useful repository! Such as the small collection of Excel, Matlab and SAS utilities and programs which can be found at www.nirpublications.com/software/