BRUKER NMR

Data Formats

User Manual

Version 004

Innovation with Integrity

NMR

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1 Data Formats

This document describes data formats used on Bruker NMR Avance (AV I-III and AV Neo) spectrometers.

1.1 Data Structure

Bruker NMR data sets are stored in a directory tree on the disc:

<data folder>/<data set name>/<EXPNO>/pdata/<PROCNO>

The folder EXPNO (the folder name is an integer number) contains the acquired raw data. The folder PROCNO (the folder name is an integer number) contains the processed spectra. Every data set may contain several PROCNO folders representing different processing schemes applied to the raw data.

The length of each part of the data set identifier is limited:

<data folder>	maximum 335 characters
<data set name>	maximum 159 characters

Please consider that additional OS specific restrictions may apply (e.g. Windows 10 has a 256 character limit for any path name).

1.2 Parameter Files

The parameter files *acqu** and *proc** containing acquisition and processing parameters, are text files (see Section of a an acqu parameter file). All parameter files ending with ‘s’ (*acqus, proc2s*...) describe the status of the dataset. The other files (acqu, proc2…) contain parameter values which will be used in the next processing or acquisition (so called foreground parameters).

Format of all parameter files corresponds to the JCAMP-DX standard. It allows the inclusion of vendor specific parameters, which are marked by the character sequence *##$*. For this reason, all parameters TopSpin parameters in the file are preceded by this sequence.

Section of an acqu parameter file:

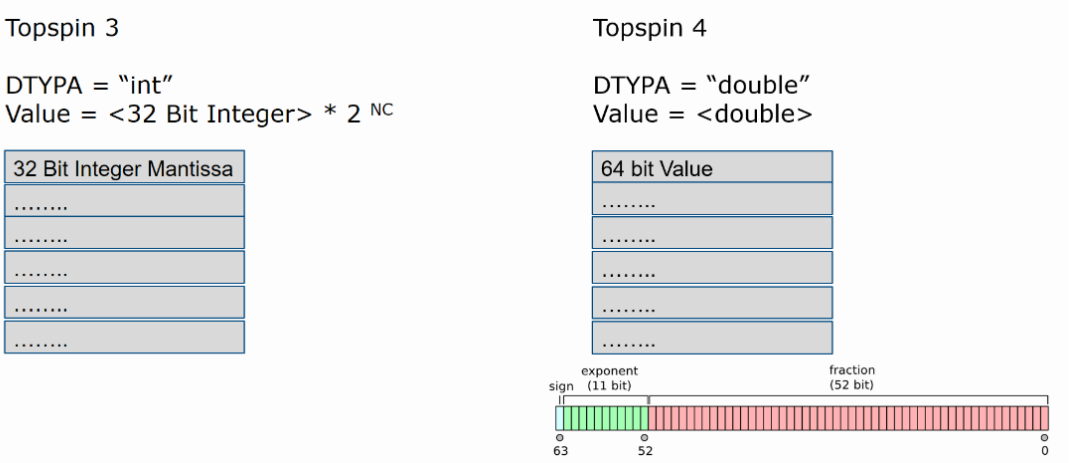
```
##TITLE= Parameter file, TopSpin 4.0.7
##JCAMPDX= 5.0
##DATATYPE= Parameter Values
##NPOINTS= 9 $$ modification sequence number
##ORIGIN= Bruker BioSpin GmbH
##OWNER= nmr
$$ 2019-12-09 14:29:46.726 +0100 nmr@CZC623791F
$$ C:/DATA/amr/400_201612 /1/acqu
##$ACQT0= 0
##$AMP= (0..31)
100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100
```

```
100 100 100 100 100 100 100 100 100 100 100 100 100 100
##$ANAVPT= 1
##$AQSEQ= 0
##$AQ_mod= 3
##$AUNM= <au_zg>
##$AUTOPOS= <>
##$BF1= 400.13
##$BF2= 400.13
##$BF3= 400.13
…… , ……
##END=
```

1.3 Raw Data

The raw data files *fid* and *ser* contain one dimensional or multi-dimensional acquired data, respectively. They consist of a sequence of acquired data point values in binary format.

The acquisition status parameter DTYPA defines, how the data values are stored. If the DTYPA is “int”, the stored value represents a mantissa of the data point value, the acquisition parameter NC is the exponent. All data points share in this case the same exponent. If DTYPA is “double”, the data points are stored as a double precision 64 bit floating number, parameter NC is not used.



On workstations with different microprocessors an integer number may be represented by a sequence of 4 bytes ordered differently. There are two common modes, *little endian* and *big endian*. The latter one is typical for MIPS and SPARC microprocessors, the former one for Intel x86 family. TopSpin stores the byte order corresponding to the acquisition data in the acquisition status parameter BYTORDA (in the file *acqus*), which may take on the value *little* or *big*. This allows TopSpin (or other software packages) to convert the data to the correct byte order, if the endian mode of the computer where the data are to be processed is different from that of the acquisition computer.

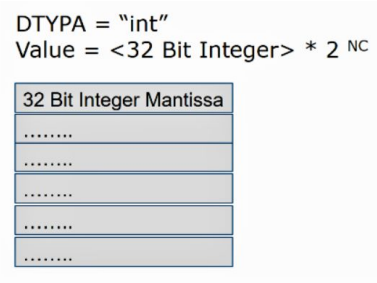
Within a FID, the data points coming from channels A and B alternate for quadrature detection data. A 1D *fid* file contains a single fid with TD points, which stored in the acquisition status parameter file *acqus*.

A 2-dimensional experiment generates a *ser* file contains TD(F1) series of FIDs, which is the parameter TD in the file *acqu2s*. Each FID in a *ser* file start at a 1024 byte block boundary, even if its size is not a multiple of 1024 bytes.

1.4 Processed Data

The processed spectra are stored in dimension-specific files as described below. They consist of a sequence of data point values in binary format.

The processing status parameter DTYPP defines how the data values are stored. If the DTYPP is 0 (“int”), the stored value represents a mantissa of the data point value, the processing status parameter NC_proc is the exponent. In this case all data points share the same exponent.



1.4.1 1D Spectra

Applying a 1D processing command to a 1D fid or reading a 1D slice from a 2D spectrum generates *processed* data. They are stored in two files *1r* and *1i*, corresponding to real and imaginary part. Like in 1D fids, the data points are stored as a sequence of data point values. Their format is given by the parameter DTYPP, the byte ordering is given by the parameter BYTORDP, both may be read from the processing status parameter file *procs*.

1.4.2 2D spectra

Like 1D spectra and raw data, 2D processed spectra are stored as a series of data point values. The spectrum real part is contained in the file *2rr*, the imaginary parts in the files *2ii*, *2ri*, *2ir*. The latter two are only present if the spectrum is phase sensitive. All files are stored in the so-called submatrix format. The submatrix dimensions are given by the status parameters XDIM contained in the files *procs* and *proc2s*. XDIM is calculated by automatically (depending on the available computer memory) so as to optimize the Fourier transform time. If the entire data set fits in memory, XDIM(F1) will be 1, and a row-wise ordering results.

On disk, a complete submatrix is stored before the next submatrix starts. The order of the data points within one submatrix is the same as the order of the submatrices within one data set, first F2 (the acquisition direction), and then F1.

The figure below shows the file structure of a processed 2D data file with the parameters SI(F2)=16 points, SI(F1)=16, XDIM(F2)4, XDIM(F1)=8.The upper left part of the figure shows the sequence of the individual data points of submatrix 1, the lower right part shows the sequence of the submatrices in the entire spectrum.

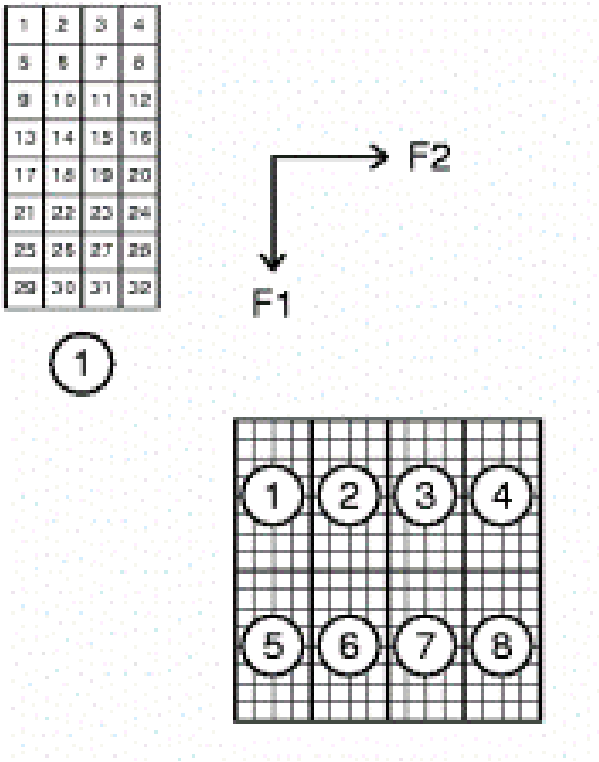


Figure 1.1: Submatrix Format

1.4.3 3D Spectra

For 3D processed data, the spectrum real part is contained in the file *3rrr*, the imaginary parts are generated according to the description of the command tf1. The files *3rrr*, *3irr*, ... are stored in the so-called subcube format, a generalization of the 2D submatrix format. The subcube dimensions are given by the status parameters XDIM contained in the files *procs*, *proc2s* and *proc3s*. XDIM is calculated by automatically (depending on the available computer memory) so as to optimize the fourier transform time. XDIM is always a power of two.

On disk, a complete subcube is stored before the next subcube starts. The order of the data points within one subcube is the same as the order of the subcubes within one data set, first F3 (the acquisition direction), then F2, and finally F1.

The figure below shows the storage order of a processed 3D data file with the parameters SI(F3)=16 points, SI(F2)=16, SI(F1)=16, XDIM(F3)=4, XDIM(F2)=8, XDIM(F1)=4. The upper left part of the figure shows the sequence of the individ- ual data points of subcube 1, the lower right part shows the sequence of the sub- cubes in the entire spectrum.

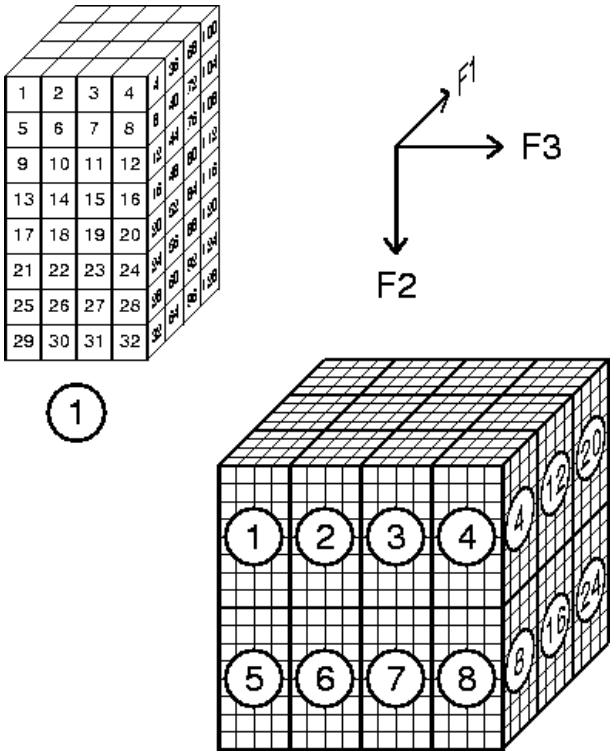


Figure 1.2: Subcube Format

1.4.4 JCAMP-DX Format

1D acquisition and processed data (files *fid, 1r, 1i*) may also be stored in text files based on the JCAMP-DX format. The initial part of such a file is similar to Section of a an acqu parameter file and contains the parameters, followed by the data section with the fid or spectrum encoded according to the option chosen when calling the JCAMP conversion command **tojdx**. For detailed information about the JCAMP format, please refer to the following literature.

- JCAMP-DX: A Standard Form for Exchange of Infrared Spectra in Computer in Readable Form.

  Robert S. McDonald and Paul A. Wilks, JR. Applied Spectroscopy 42, Number 1, 1988
- Generic JCAMP-DX, Version 5.0 Draft 1.0 February 28, 1991

  Robert S. McDonald, JCAMP-DX subcommittee, 9 Woodside Drive, Burnt Hills, NY 12027, USA
- JCAMP-DX NMR Standard

  Dr. A. N. Davies, ISAS, Institut für Spektrochemie, Dortmund, Germany (private comm.)

1.5 Pulse Shapes

Pulse shapes (waveforms) are stored in the directory <*XWINNMRHOME*>*/exp/stan/nmr/lists/wave/* in ASCII format conforming to JCAMP-DX. The example below shows a section of a shape file. The data points represent the amplitude and phase values.

Bruker shape file format:

```
##TITLE= sm. comp. Chirp: 60kHz, 2ms
##JCAMP-DX= 5.00 Bruker JCAMP library
##DATA TYPE= Shape Data
##ORIGIN= Bruker BioSpin GmbH
```

```
##OWNER= <demo>
##DATE= 2005/09/22
##TIME= 18:40:13
##$SHAPE_PARAMETERS= Type: CompositeSmoothedChirp Add Const. Phase
-84.0
##MINX= 0.000000E00
##MAXX= 1.000000E02
##MINY= 1.110750E-01
##MAXY= 3.599617E02
##$SHAPE_EXMODE= CompositeAdiabatic
##$SHAPE_TOTROT= 1.800000E02
##$SHAPE_TYPE= Refocussing
##$SHAPE_USER_DEF=
##$SHAPE_REPHFAC=
##$SHAPE_BWFAC= 8.099400E01
##$SHAPE_BWFAC50=
##$SHAPE_INTEGFAC= 2.558317E-02
##$SHAPE_MODE= 0
##NPOINTS= 4000
##XYPOINTS= (XY..XY)
0.000000E00, 1.833013E02
7.893367E-01, 1.779122E02
……, ……
##END=
```

2 Contact

Manufacturer

Bruker BioSpin GmbH
Silberstreifen 4
D-76287 Rheinstetten
Germany

E-Mail: *nmr-support@bruker.com*
http://www.bruker.com
WEEE DE43181702

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