# Chapter 15

# File Formats

## 15.1 Parameter Files

The parameter files *acqu**, *proc**, and *meta** containing acquisition, processing, and plot parameters, respectively, are text files (see Figure 15.1). Their format corresponds to the so-called JCAMP-DX standard. It allows the inclusion of user specific parameters, which are marked by the character sequence *##$*. For this reason, all parameters XWIN-NMR parameters in the file are preceded by this sequence.

## 15.2 Acquisition Data

The files *fid* and *ser* contain one dimensional or multi-dimensional acquisition data, respectively. They consist of a sequence of 32 bit integer numbers in binary format. 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 and Bruker X32. XWIN-NMR 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 XWIN-NMR (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 proc-

```
##TITLE= Parameter file,  XWIN-NMR version 1.0
##JCAMPDX= 5.0
##DATATYPE=  Parameter Values
##ORIGIN=XWIN-NMR
##OWNER= jos
$$ Mon Jul 18 16:30:18 1994
$$ File: /u/data/guest/nmr/IQUIN128/1/acqu
##$AQ_mod= 1
##$D= (0..31)
3e-06 2 0.071 0.002 0.015 0.001 0.0005 1.5 10 0.7 0 0 0 0 0 0 0 0 0 0
##$DR= 12
##$LOCNUC= <2H>
##$LOCSHFT= no
##$NS= 8
##$NUC1= <1H>
##$PULPROG= <zg>
##$PW= 4.5
##$RO= 20
##$SW_h= 826.719576719577
##$TD= 131072
##$TE= 303
##END=
```

**Figure 15.1** Section of a an *acqu* parameter file

essed is different from that of the acquisition computer.

Within an 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(F2) points, which is the time domain size TD stored in the acquisition status parameter file *acqus*. A *ser* file contains TD(F1) 1D fids, which is the parameter TD in the file *acqu2s*. Each 1D fid in a *ser* file start at a 1024 byte block boundary, even if its size is not a multiple of 1024 bytes (corresponding to 256 data points).

## 15.3 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*, corre-

sponding to real and imaginary part. Like in 1D fids, the data points are stored as a sequence of 32 bit integers. Their byte ordering is given by the parameter BYTORDP, which may be read from the processing status parameter file *procs*.

## 15.4 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 Figure 15.1 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. Fore detailed information about the JCAMP format, please refer to the following literature.

**1.** 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

**2.** Generic JCAMP-DX, Version 5.0 Draft 1.0 February 28, 1991
Robert S. McDonald, JCAMP-DX subcommitte, 9 Woodside Drive, Burnt Hills, NY 12027, USA

**3.** JCAMP-DX NMR Standard
Dr. A. N. Davies, ISAS, Institut für Spektrochemie, Dortmund, Germany (private comm.)

## 15.5 2D spectra

Like 1D spectra and acquisition data, 2D processed data are stored as 32 bit integers. 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.

Figure 15.2 shows the file structure of a processed 2D data file with the

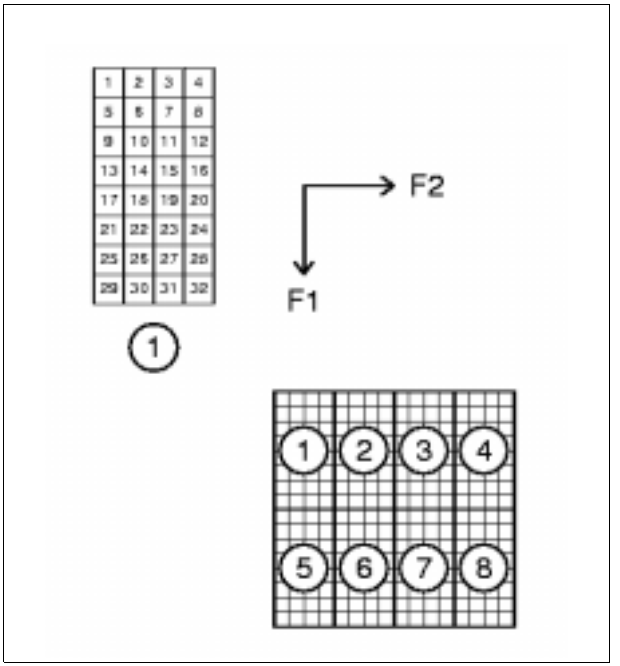


**Figure 15.2** Submatrix format

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.

## 15.6 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 calcu-

lated 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.

Figure 15.3 shows the storage order of a processed 3D data file with the

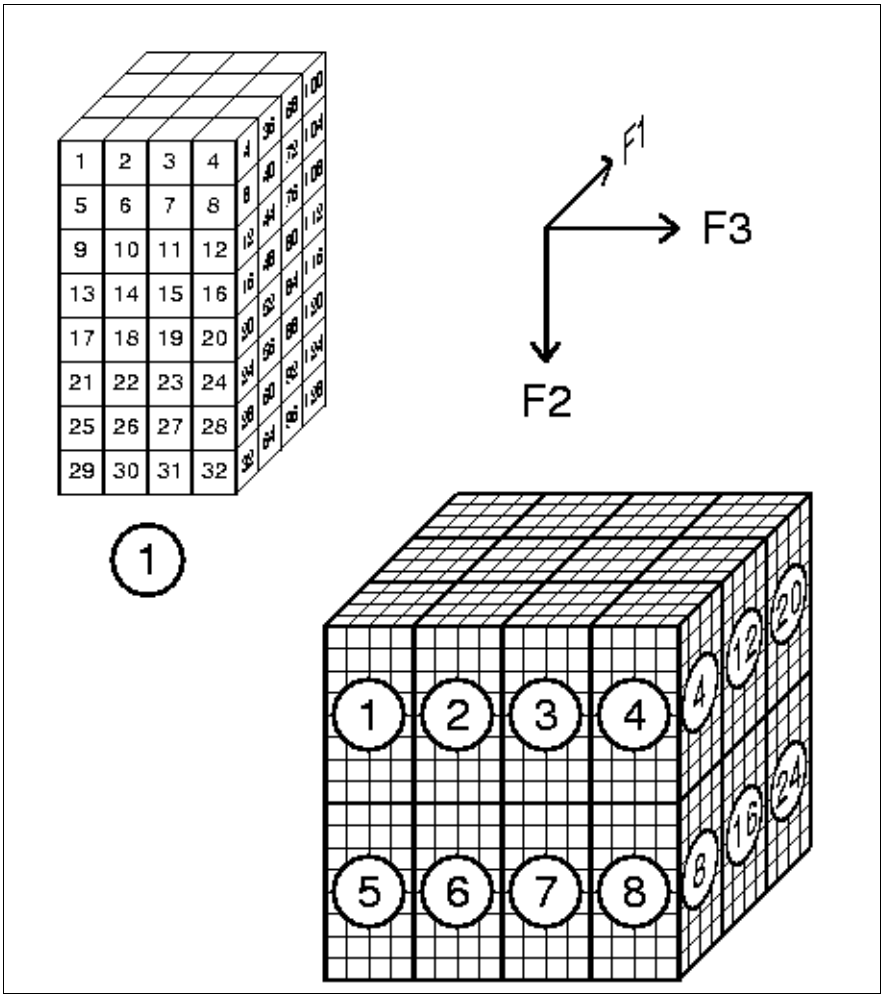


**Figure 15.3** Subcube format

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 individual data points of subcube 1, the lower right part shows the sequence of the subcubes in the entire spectrum.

## 15.7 Pulse Shapes

### 15.7.1 XWIN-NMR 2.0 and later

Pulse shapes are stored in the directory *XWINNMRHOME/exp/stan/nmr/lists/wave/* in ASCII format conforming to JCAMP-DX. Table 15.1 shows a section of a shape file. The data points represent the amplitude and phase values.

### 15.7.2 XWIN-NMR versions earlier than 2.0

Pulse shapes are stored in the directory *XWINNMRHOME/exp/stan/nmr/lists/wave/*. There are two types of data formats, a binary one required by XWIN-NMR for the execution of shaped pulses, generated by the program *shape*, and a text format which can be read into *shape* by the command ar, and stored back in binary format by w for use with XWIN-NMR.

**Text Format**

The text format is particularly useful if you want to generate own shapes by a suitable program. Figure 15.4 shows an example. The file starts with the text RFVERSION_F, then the pulse shape follows. The first column contains the amplitudes, the second one the corresponding phases. If the phases are omitted, the following rule applies: the phases are set to 0 if the amplitudes are positive, and to 180 degrees if negative. Phases are specified in degrees in the range 0-360 (floating point numbers are legal). A file must not contain more than 32768 lines. Amplitudes and phases are separated by a space, tabulator, or comma.

Relative power values may range from 0-100. If a value in the file exceeds 100, it will be rescaled to 100 during execution. All other points will be rescaled accordingly. Values less than 100 will not be rescaled.

**Binary Format**

The binary file format of shape files is as follows:

```
##TITLE= /u//exp/stan/nmr/lists/wave/CosSinc
##JCAMP-DX= 5.00 $$ Bruker JCAMP library
##DATA TYPE= Shape Data
##ORIGIN= Bruker Analytik GmbH
##OWNER= <guest>
##DATE= 96/09/21
##TIME= 12:11:57
##MINX= 0.000000e+00
##MAXX= 9.956761e+01
##MINY= -9.552316e+01
##MAXY= 1.794392e+02
##$SHAPE_EXMODE= None
##$SHAPE_TOTROT= 0.000000e+00
##$SHAPE_BWFAC= 0.000000e+00
##$SHAPE_INTEGFAC= 2.052226e-03
##$SHAPE_MODE= 4
##NPOINTS= 256
##XYPOINTS= (XY..XY)
0.000000e+00, -1.869338e-01
7.815741e-01, 1.794392e+02
1.522001e+00, 1.790653e+02
2.671471e+00, 1.783176e+02
2.985925e+00, 1.779437e+02
3.074292e+00, 1.775699e+02
2.907826e+00, 1.771960e+02
2.468165e+00, 1.768221e+02
1.748423e+00, 1.764483e+02
1.689626e+01, -8.412024e+00
....................., .....................
##END=
```

**Table 15.1** JCAMP-DX shape file format

- **Header**: consists of 256 32 bit float words.
  1. word 1 contains file type information:
     371242.0 (= GRADVERSION_F) or 18906.0 (= RFVERSION_F)
  2. word 2 contains # of amplitudes (=amps) stored

```
RFVERSION_F
10  0
20  90
30  180
40  270
50  360
```

**Figure 15.4** old ASCII shape file format

3. word 3 contains # of phases (=phas) stored
4. word 4 to word 256 are unused

- **Data**: consists of (amps + phas) 32 bit float words.
  1. *RFVERSION*: pairs of phases and ampitudes: phases (in degrees) from 0.0 to 360.0 and amplitudes from 0.0 to 100.0 %. Phases are always stored as first value followed by the corresponding amplitude.
  2. *GRADVERSION*: only amplitudes are stored (values from 0.0 up to 100.0 %). Phases allowed are 0.0 and 180.0 degrees. If the phase is 180.0 degrees, the stored amplitude is negated. No phases are stored in the file.

The maximum size of amplitudes (for GRADVERSION) or pairs of amplitudes and phases (=RFVERSION) is 32K (or 32768 points/pairs).

## 15.8 Other files

Many other files play a role in XWIN-NMR, such as integral range files, peak lists etc. They are described in the chapter *The File Menu*, or in conjunction with the command generating them.