Sequence Editor Specification

1. Sequence definition
2. Signal Display
3. Post Processing
4. HW interface through a spectrometer.dll (COM)
5. Shim– TBD
6. Appendix A - NTNMR File Format
7. Sequence Definition
   1. Dashboard – Defines the parameter that will be used in the sequence (e.g. AcqPoints)
   2. All fields in the dashboard are required including the “Manual Variable” definition that enables to define a new variable that will be used in the sequence (refer to the sequence tab and the +V icon on the left bar)
   3. The output of the sequence editor is a sequence file (tnt). FileformatdescribedinAppendix A
   4. The sequence file must be coupled to a “Sequence Parameters File” that contains the parameters that will be used when compiling the sequence
   5. Since the sequence editor is used to run the spectrometer and display acquired signals, we need to add an easy way to modify sequence parameters at runtime (e.g. defining per each parameter an increment/decrement step, and when the user selects the parameter, he gets an up/down small buttons next to the parameter)
   6. From the left bar – only 2 buttons are required – “add variable”, and “setup dashboard”
   7. If multiple sequences are loaded, then the dashboard displays theparameters of the active signal
   8. Refer to NTNMR Reference Guide.pdf chapter 4.4 for a list of dashboard parameters
   9. Each line in the sequence definition, represent a single channel and enables to define the activity in this channel in the timeline (Полный список каналов)
   10. Sequence Editing – all the icons on the left bar are N/A except for “Toggle Text Mode” and “Edit Labels” (Непонятно какие кнопки должны быть)
   11. Chapter 10 – “Pulse Sequences” should be implemented
8. Signal Display (Каким хером сигнал строить)
   1. Only FID Display – Signal in time domain (непонятно что за вид такой)
   2. nDdisplayis N/A – discard chapter 8 (несовсем понятно)
   3. Signal export format – TBD (что за формат и где описание)
   4. Enable zooming
9. Post Processing
   1. No processing functionality is required – signal should be displayed in time domain only. (непонятно что это значит)
   2. Chapter 6.4-6.9 , Chapter 7 is N/A
10. HW interface through a spectrometer.dll (COM)
    1. The DLL will be developed by NATIX and will provide the functionality described below.
    2. The DLL will be used for acquiring a new signal from HW (we will also provide simulation mode so it can be used without HW)
11. Acquisition Commands
    1. Abort
    2. Check Acquisition
    3. Go
    4. Stop
    5. Zero and Go
12. Data Organization Commands
    1. DigitalCorrect
    2. EchoZeroFill
    3. Export
    4. ExtractRecord
    5. ExtractRecordToFile
    6. GetDataSize
    7. GetNDSize
    8. LeftShift
    9. NDComplexTranspose
    10. NDTranspose
    11. ReadFirstHalf
    12. ReadSecondHalf
    13. ReSetDimensionInfo
    14. ReSetMatrix
    15. ReverseSpectrumColumns
    16. ReverseSpectrumRows
    17. RightShift
    18. SortDataPoints
    19. Transpose
    20. ZeroFill
    21. ZeroImaginary
13. File I/O Commands
    1. Copy
    2. Save
    3. SaveAs
    4. SaveAsJpg
    5. CloseActiveFile
    6. CloseFile
    7. GetActiveDocPath
    8. OpenFile
14. Transform Commands
    1. FFT
15. Dashboard/Parameter Commands
    1. GetParameterPageList
    2. GetParameterListInPage
    3. LoadParametersFromFile
    4. RemoveAllParameterPages
    5. RemoveParameterPage
    6. SaveParameterSetupToFile
    7. SaveParametersToFile
    8. SetActiveParameterPage
    9. SetParameterListInPage
16. Hardware Commands
    1. CreateHWInterface
    2. GetLatchedData
    3. RepeatScan
    4. Reset
    5. SetLatchedData
    6. SoftStop
17. Miscellaneous Commands
    1. GetDocumentList
    2. GetUploadDataMode
    3. HideWindow
    4. NewDataWindow
    5. Quit
    6. ReloadConfig
    7. SetUploadDataMode
    8. ShowWindow
18. Printing Commands
    1. AddActiveDocToPrintPreview
    2. ClosePrintPreview
    3. LoadPrintPreviewTemplate
    4. OpenPrintPreview
    5. PrintFromPreview

Appendix A

NTNMR File Format (80114)

**Quick Start:**

The following is the essential information to extract the data from a \*.tnt data file.

See the following pages for details about the file format.

Bytes to skip to get to the data: 1056

Data format:

RIRIRIRI, blocks in linear order according to how they were collected

Example:

To read a 1D data file with 2048 pointsspecifiyanoffsetof 1056 bytes, a data length of 2048, and a format of R, I, R, I, R…

2D data is stored in a serial fashion. To read a 2D file the data length would be specified as (#records \* Points 1D).

**Data Format Outline**

(see below for TECMAG and TECMAG2 data structures)

|  |  |  |  |
| --- | --- | --- | --- |
| **Item** | **Size (bytes)** | **Offset** | **Comment** |
| “TNT1.000” version ID | 8 | 0 |  |
| ‘TMAG’ tag | 4 | 8 |  |
| BOOLeanvalue | 4 | 12 |  |
| lengthofTecmagstruct | 4 | 16 | usually 1024 |
| TECMAG structure | 1024 | 20 |  |
| ‘DATA’ tag | 4 | 1044 |  |
| BOOLean | 4 | 1048 |  |
| length of data | 4 | 1052 |  |
| actual data (floating point - 4  byteinreal/imagpairs) | data\_offset = 2 \* 4 \* npts[0]  \* npts[1] \* npts[2] \* npts[3] | 1056 |  |
| ‘TMG2’ tag | 4 | 1056 + data\_offset |  |
| BOOLean | 4 | 1056 + data\_offset + 4 |  |
| lengthof TECMAG2 struct | 4 | 1056 + data\_offset + 8 | usually 2048 |
| TECMAG2 structure | 2048 | 1056 + data\_offset + 12 |  |
| ‘PSEQ’ tag | 4 | 1056 + data\_offset + 2060 |  |
| BOOLean | 4 | 1056 + data\_offset + 2064 |  |
| Sequence | variable |  |  |
|  |  |  |  |
| **Optional Sections:** | Not necessarily in any order |  |  |
| **Peaks:** |  |  |  |
| ‘PEAK’ tag | 4 |  |  |
| BOOLean | 4 |  |  |
| number of peaks | 4 |  |  |
| sizeofofpeakinfo | 8 (long + BOOL) | (longpeak\_point, BOOL manually\_chosen) | |
| peak info \* number of peaks | 8 \* number of peaks |  |  |
|  |  |  |  |
| **Integrals:** |  |  |  |
| ‘INTG’ tag | 4 |  |  |
| BOOLean | 4 |  |  |
| number of integrals | 4 |  |  |
| size of integral info | 28 (4 float + 3 long) | (float slope, floatcurvature, floatfudge\_factor,  floatmultiplier, longstart\_point, longend\_point,  longbounds\_rect.bottom | |
| integral info \* number of  integrals | 28 \* number of integrals |  |  |
|  |  |  |  |
| **Comments**: |  |  |  |
| ‘COMM’ tag | 4 |  |  |
| BOOLean | 4 |  |  |
| length of string | 4 |  |  |
| comment string | length of string |  |  |

TECMAG Structure

Number of points and scans in all dimensions:

Type ID Size (bytes) Desc

long npts[4]; 16 points requested 1D, 2D, 3D, 4D

long actual\_npts[4]; 16 points completed in each dimension

(actual\_npts[0] is not really used)

long acq\_points; 4 acq\_points will be number of points to acquire

during one acquisition icon in the sequence

(which may be smaller than npts[0])

long npts\_start[4]; 16 scan or pt on which to start the acquisition

long scans; 4 scans 1D requested

long actual\_scans; 4 scans 1D completed

long dummy\_scans; 4 number of scans to do prior to

collecting actual data

long repeat\_times; 4 Number of times to repeat scan

long sadimension; 4 signal average dimension

long samode; 4 sets behavior of the signal averager for the

dimension specified in S.A. Dimension

char space1[0]; 0

----

76

Field and frequencies:

double magnet\_field; 8 magnet field

double ob\_freq[4]; 32 observe frequency

double base\_freq[4]; 32 base frequency

double offset\_freq[4]; 32 offset from base

double ref\_freq; 8 reference frequency for axis

calculation (used to be freqOffset)

double NMR\_frequency; 8 absolute NMR frequency

short obs\_channel; 2 observe channel defalut = 1;

char space2[42]; 42

----

164

Spectral width, dwell and filter:

double sw[4]; 32 spectral width in Hz

double dwell[4]; 32 dwell time in seconds

double filter; 8 filter

double experiment\_time; 8 time for whole experiment

double acq\_time; 8 acquisition time - time for acquisition

double last\_delay; 8 last delay in seconds

short spectrum\_direction; 2 1 or -1

short hardware\_sideband; 2

short Taps; 2 number of taps on receiver filter

short Type; 2 type of filter

BOOL bDigRec; 4 toggle for digital receiver

long nDigitalCenter; 4 number of shift points for digital receiver

char space3[16]; 16

----

128

Hardware settings:

short transmitter\_gain; 2 transmitter gain

short receiver\_gain; 2 receiver gain

short NumberOfReceivers; 2 number of Rx in MultiRx system

short RG2; 2 receiver gain for Rx channel 2

double receiver\_phase; 8 receiver phase

char space4[4]; 4

-----

20

Spinning speed information:

unsigned short set\_spin\_rate; 2 set spin rate

unsigned short actual\_spin\_rate; 2 actual spin rate read from the meter

----

4

Lock information:

short lock\_field; 2 lock field value (might be Bruker specific)

short lock\_power; 2 lock transmitter power

short lock\_gain; 2 lock receiver gain

short lock\_phase; 2 lock phase

double lock\_freq\_mhz; 8 lock frequency in MHz

double lock\_ppm; 8 lock ppm

double H2O\_freq\_ref; 8 H1 freq of H2O

char space5[16]; 16

----

48

VT information:

double set\_temperature; 8 non-integer VT

double actual\_temperature; 8 non-integer VT

----

16

Shim information:

double shim\_units; 8 shim units (used to be SU)

short shims[36]; 72 shim values

double shim\_FWHM; 8 full width at half maximum

----

88

Brukerspecificinformation:

short HH\_dcpl\_attn; 2 decoupler attenuation

(0..63 or 100..163); receiver gain is above

short DF\_DN; 2 decoupler

short F1\_tran\_mode[7]; 14 F1 Pulse transmitter switches

short dec\_BW; 2 decoupler BW

----

20

char grd\_orientation[4]; 4 gradient orientation

long LatchLP; 4 990629JMB values for lacthed LP board

double grd\_Theta; 8 990720JMB gradient rotation angle Theta

double grd\_Phi; 8 990720JMB gradient rotation angle Phi

char space6[264]; 264 space for the middle

Timevariables

CTime start\_time; 4 starting time

CTime finish\_time; 4 finishing time

CTimeSpan elapsed\_time; 4 projected elapsed time

textbelowandvariables above

----

300

Text variables: // 96 below

char date[32]; 32 experiment date

char nucleus[16]; 16 nucleus

char nucleus\_2D[16]; 16 2D nucleus

char nucleus\_3D[16]; 16 3D nucleus

char nucleus\_4D[16]; 16 4D nucleus

char sequence[32]; 32 sequence name

char lock\_solvent[16]; 16 Lock solvent

char lock\_nucleus[16]; 16 Lock nucleus

----

160

TECMAG Structure total => 1024

TECMAG2 Structure

Display Menu flags:

Type ID Size Desc

BOOL real\_flag; 4 displayreal data

BOOL imag\_flag; 4 displayimaginary data

BOOL magn\_flag; 4 displaymagnitude data

BOOL axis\_visible; 4 displayaxis

BOOL auto\_scale; 4 autoscale mode on or off

BOOL line\_display; 4 TRUE for lines, FALSE for points

BOOL show\_shim\_units; 4 displayshim units on the data area or not

----

28

Option Menu flags:

BOOL integral\_display; 4 integrals turned on? - but not swap area

BOOL fit\_display; 4 fits turned on? - butnotswap area

BOOL show\_pivot; 4 showpivot point on screen; only used

during interactive phasing

BOOL label\_peaks; 4 show labels on the peaks?

BOOL keep\_manual\_peaks; 4 keepmanual peaks when re-applying

peak pick settings?

BOOL label\_peaks\_in\_units; 4 peaklabel type

BOOL integral\_dc\_average; 4 usedc average for integral calculation

BOOL integral\_show\_multiplier; 4 showmultiplier on integrals that are scaled

BOOL Boolean\_space[9]; 36

----

68

Processing flags:

BOOL all\_ffts\_done[4]; 16

BOOL all\_phase\_done[4]; 16

----

32

Vertical display multipliers:

double amp; 8 amplitude scale factor

double ampbits; 8 resolution of display

double ampCtl; 8 amplitude control value

long offset; 4 vertical offset

----

28

grid\_and\_axis axis\_set; 256 see Grid and Axis Structure below

short display\_units[4]; 8 display units for swap area

long ref\_point[4]; 16 for use in frequency offset calcs

double ref\_value[4]; 32 for use in frequency offset calcs

long z\_start; 4 beginning of data display

(range: 0 to 2 \* npts[0] - 2)

long z\_end; 4 end of data display (range: 0 to 2 \* npts[0] - 2)

long z\_select\_start; 4 beginning of zoom highlight

long z\_select\_end; 4 end of zoom highlight

long last\_zoom\_start; 4 last z\_select\_start - not used yet (4/10/97)

long last\_zoom\_end; 4 last z\_select\_end - not used yet (4/10/97)

long index\_2D; 4 in 1D window, which 2D record we see

long index\_3D; 4 in 1D window, which 3D record we see

long index\_4D; 4 in 1D window, which 4D record we see

----

92

long apodization\_done[4]; 16 masked value showing which processing

has been done to the data; see constants.h for values

double linebrd[4]; 32 line broadening value

double gaussbrd[4]; 32 gaussian broadening value

double dmbrd[4]; 32 double exponential broadening value

double sine\_bell\_shift[4]; 32 sine bell shift value

double sine\_bell\_width[4]; 32 sine bell width value

double sine\_bell\_skew[4]; 32 sine bell skew value

long Trapz\_point\_1[4]; 16 first trapezoid point for trapezoidal apodization

long Trapz\_point\_2[4]; 16 second trapezoid point for

trapezoidalapodization

long Trapz\_point\_3[4]; 16 third trapezoid point for trapezoidal

apodization

long Trapz\_point\_4[4]; 16 fourth trapezoid point for trapezoidal apodization

double trafbrd[4]; 32 Traficante-Ziessow broadening value

long echo\_center[4]; 4 echo center for all dimensions

----

320

long data\_shift\_points; 4 number of points to use in

left/right shift operations

short fft\_flag[4]; 8 fourier transform done?

false if time domain, true if frequency domain

double unused[8]; 64

long pivot\_point[4]; 16 for interactive phasing

double cumm\_0\_phase[4]; 32 cummulative zero order phase applied

double cumm\_1\_phase[4]; 32 cummulative first order phase applied

double manual\_0\_phase, 8 used for interactive phasing

double manual\_1\_phase; 8 used for interactive phasing

double phase\_0\_value, 8 last zero order phase value

applied (not necessarily equivalent to

cummulative zero order phase)

double phase\_1\_value; 8 last first order phase value applied

(not necessarily equivalent to cummulative

first order phase)

double session\_phase\_0, 8 used during interactive phasing

double session\_phase\_1; 8 used during interactive phasing

----

204

long max\_index; 4 index of max data value

long min\_index; 4 index of min data value

float peak\_threshold, 4 threshold above which peaks are chosen

float peak\_noise; 4 minimum value between two points that are

above the peak threshold to distinguish two

peaks from two points on the same peak

short integral\_dc\_points; 2 number of points to use in integral

calculation when dc average is used

short integral\_label\_type; 2 how to label integrals, see constants.h

float integral\_scale\_factor; 4 scale factor to be used in integral draw

long auto\_integrate\_shoulder; 4 number of points to determine

where integral is cut off

double auto\_integrate\_noise; 8 when average of shoulder points is

under this value, cut off integral

double auto\_integrate\_threshold; 8 threshold above which a peak

is chosen in auto integrate

long s\_n\_peak; 4 peak to be used for signal to noise calculation

long s\_n\_noise\_start; 4 start of noise region for

signal to noise calculation

long s\_n\_noise\_end; 4 end of noise region for signal to noise calculation

float s\_n\_calculated; 4 calculated signal to noise value

----

60

long Spline\_point[14]; 56 points to be used for

spline baseline fix calculation

short Spline\_point\_avr; 2 for baseline fix

long Poly\_point[8]; 32 points for polynomial baseline fix calculation

short Poly\_point\_avr; 2 for baseline fix

short Poly\_order; 2 what order polynomial to use

----

94

Blank Space:

char space[610]; 610

Text variables:

char line\_simulation\_name[32]; 32

char integral\_template\_name[32]; 32

char baseline\_template\_name[32]; 32

char layout\_name[32]; 32

char relax\_information\_name[32]; 32

char username[32]; 32

char user\_string\_1[16]; 16

char user\_string\_2[16]; 16

char user\_string\_3[16]; 16

char user\_string\_4[16]; 16

----

256

TECMAG2 Structure Total => 2048

Grid and Axis Structure

Type ID Size(bytes) Desc

double majorTickInc[TOTAL\_UNIT\_TYPES]; 8 \* 12 = 96 Increment between major ticks

short minorIntNum[TOTAL\_UNIT\_TYPES]; 2 \* 12 = 24 Number of intervals between major ticks

(minor ticks is one less than this)

short labelPrecision[TOTAL\_UNIT\_TYPES]; 2 \* 12 = 24 Number of digits after the decimal point

double gaussPerCentimeter; 8 Used for calculation of distance

axis in frequency domain

short gridLines; 2 Number of horizontal grid lines to

be shown in data area

short axisUnits; 2 Type of units to show - see constants.h

BOOL showGrid; 4 Show or hide the grid

BOOL showGridLabels; 4 Show or hide the labels on the grid lines

BOOL adjustOnZoom; 4 Adjust the number of ticks and the

precisionwhenzoomedin

BOOL showDistanceUnits; 4 whetherto show frequency or distance

units when in frequency domain

char axisName[32]; 32 file name of the axis (not used as of 4/10/97)

char space[52]; 52

----

256

**Pulse Sequence:**

‘PSEQ’ tag 4

BOOLean 4

SequenceID 8 “1.04 BIN”

Filename Length 4

File Name Length

Number of Rows 4

Number of Columns 4

**Sequence Rows: Number of Rows \* (variable length)**

Number of Columns 4

Address 4

BitLength 4

Icon Library Type 4

Visible Flag 4

Private Data 4

Group 4

DefalutStringLength 4

DefalutString Length

LabelStringLerngth 4

Label String Length

**Sequence Events Number of Columns \* (Variable length)**

Data String Length 4

Data String Length

0D Table Name Length 4

0D Table Name Length

0D Table Flag 4

1D Table Name Length 4

1D Table Name Length

1D Table Flag 4

2D Table Name Length 4

2D Table Name Length

2D Table Flag 4

3D Table Name Length 4

3D Table Name Length

3D Table Flag 4

4D Table Name Length 4

4D Table Name Length

4D Table Flag 4

**Sequence Tables: Number of Tables \* variable length**

Table Name Length 4

Table Name Length

Table Entry Length 4

Table Entry Length

Increment Operation Length 4

Increment Operation Length

Increment Value Length 4

Increment Value Length

Increment Scheme Length 4

Increment Scheme Length

Repeat Time 4

Type Of Table 4

Dimension 4

StepsPer360Cycle 4

Use As Increment List 4 (BOOL)

ValueType 4 (int)

**Sequence Parameter Pages**

number of pages 4

**Parameters Pages Number of Pages \* variable length**

Page Name Length 4

Page Name Length

Number on Page 4

**Parameter Names Number on Page \* variable length**

Parameter Name Length 4

Parameter Name Length

**Sequence Parameters**

Number of Parameters 4

**Parameters Number of Parameters \* variable length**

Parameter Name Length 4

Parameter Name Length

Value String Length 4

Value String Length

Parameter Type 4

Minimum String Length 4

Minimum String Length

MaximumStriongLength 4

Maximum String Length

ReadOnlyFlag 4

**Sequence comment**

‘SEQC’ tag 4

Length of Comment 4

Comment Length

long Count = m\_SeqComment.GetLength();