TNMR File Format (100630)

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 points specifiy an offset of 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	
BOOLean value	4	12	
length of Tecmag struct	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 byte in real/imag pairs)	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	
length of 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		
sizeof of peak info	8 (long + BOOL)	(long peak_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, float curvature, float fudge_factor, float multiplier, long start_point, long end_point, long bounds_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
		----	
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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

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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	

Bruker specific information:

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

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                                                        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

Time variables
CTime         start_time;                      4         starting time
CTime         finish_time;                     4         finishing time
CTimeSpan     elapsed_time;                    4         projected elapsed time
                                                         text below and variables 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
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TECMAG2 Structure

Display Menu flags:

Type	ID	Size	Desc
BOOL	real_flag;	4	display real data
BOOL	imag_flag;	4	display imaginary data
BOOL	magn_flag;	4	display magnitude data
BOOL	axis_visible;	4	display axis
BOOL	auto_scale;	4	auto scale mode on or off
BOOL	line_display;	4	TRUE for lines, FALSE for points
BOOL	show_shim_units;	4	display shim units on the data area or not
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		28	

Option Menu flags:

BOOL	integral_display;	4	integrals turned on? - but not swap area
BOOL	fit_display;	4	fits turned on? - but not swap area
BOOL	show_pivot;	4	show pivot point on screen; only used during interactive phasing
BOOL	label_peaks;	4	show labels on the peaks?
BOOL	keep_manual_peaks;	4	keep manual peaks when re-applying peak pick settings?
BOOL	label_peaks_in_units;	4	peak label type
BOOL	integral_dc_average;	4	use dc average for integral calculation
BOOL	integral_show_multiplier;	4	show multiplier 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 trapezoidal apodization
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
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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 precision when zoomed in
BOOL	showDistanceUnits;	4	whether to 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	
Defalut String Length	4	
Defalut String	Length	
Label String Lerngth	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)
Value Type	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
Maximum Striong Length	4
Maximum String	Length
ReadOnly Flag	4

Sequence comment

'SEQC' tag	4

Length of Comment   4
Comment   Length
long Count = m_SeqComment.GetLength();