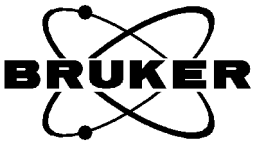
AU PROGRAMS

Reference Manual



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Chapter 1

Introduction

1.1 What are AU programs?

AU programs can be considered as user defined XWIN-NMR commands. Any repetitive task is most effectively accomplished through an AU program. All commands which can be entered on the XWIN-NMR command line can also be entered in an AU program in the form of macros. This includes selecting and changing datasets, reading and setting parameters, starting acquisitions, processing data and plotting the result. A simple AU program is nothing else than a sequence of such macros which execute the corresponding XWIN-NMR commands. However, AU programs may also contain C-language statements. In fact, an AU program is a C-program because all AU macros are translated to C-statements. XWIN-NMR automatically compiles AU programs to executable binaries, using a C-compiler.

XWIN-NMR offers two other ways of creating user defined commands: XWIN-NMR macros (not to be confused with AU macros) and Tcl/Tk scripts.They differ from AU programs in that they do not need to be compiled.

1.2 What is new in XWIN-NMR 3.1

Standard processing AU programs, like ***proc_1d*** contain the AUTOPLOT macro for plotting whereas in XWIN-NMR 3.0 and older, the PLOT macro was used. How-

ever, AU programs that contain PLOTX macros; are still used in the original form. The old AU programs, using PLOT macro, are still available under the names ***p_**. For example, the standard 1D processing AU program is available as:

proc_1d - contains the AUTOPLOT macro
p_1d - contains the PLOT macro

ICON-NMR 3.1 automatically uses AU programs with the AUTOPLOT macro.

Processing AU programs that contain the AUTOPLOT macro can be used with one of the options ***e***, ***h*** or ***t***. They cause AUTOPLOT to store the plot as a postscript file. For example, the AU program ***proc_1d*** can be enter as:

proc_1d - prints to the printer defined in the layout

proc_1d e - also prints to a postscript file in the dataset procno

proc_1d h - also prints to a postscript file in the users home directory

proc_1d t - also prints to a postscript file in the TEMP directory

(see also the header of the AU program ***plot_to_file***)

ICON-NMR 3.1 can be configured to use the call the AU programs with the ***e*** option (***Configuration → Automation Driver Engine → Master Switches → Generate Spectrum Print-Out ...***). Note that if ***Datamail*** in the ***User Settings → User Manager*** is checked, the plot is not stored but sent as an Email.

The commands ***wsr*** and ***wsc*** take an extra argument, the experiment number. The corresponding AU macros must be specified as follows:

WSR(row, procno, expno, name, user, disk)

WSC(column, procno, expno, name, user, disk)

The new command ***rser2d*** exists. The corresponding AU macro can be used as follows:

RSER2D(direction, plane, expno, procno)

1.3 Quick reference to using AU programs

Bruker delivers a library of standard AU programs with XWIN-NMR. After XWIN-NMR has been installed you must do the following in order to use them:

1. Run ***expinstall*** once to install all AU programs

2. Run ***compileall*** once to compile all AU programs
3. Enter the name of an AU program to execute it

Furthermore, you can write you own AU programs in the following way:

1. Enter ***edau <name>***
   The file <name> will be opened with a text editor
2. Do one of the following:
   - Write your own AU program from scratch
   - Read in an existing AU program and modify it according to your needs
3. Save the result and exit from the editor.
   Press **return** to answer the question about compilation.
4. Enter the name of the AU program to execute it.

After you have installed a new version of XWIN-NMR, you must run ***expinstall*** and ***compileall*** again to install and compile both Bruker's and your own AU programs.

1.4 Installing and compiling AU programs

When you have installed a new version of XWIN-NMR, you must install the library AU programs once by executing the XWIN-NMR command ***expinstall***. Your own AU programs which you created under a previous version of XWIN-NMR are still available, they only need to be re-compiled.

After running ***expinstall***, there are 5 different commands to compile AU programs:

- ***compileall***
  compile all library and user-defined AU programs
- ***cplbruk <name>*** or ***cplbruk all***
  compile one or all Bruker AU programs
- ***cpluser <name>*** or ***cpluser all***
  compile one or all user-defined AU programs
- ***edau <name>***
  create (or view) and compile one AU program
- ***xau <name>***
  compile and execute one AU program

1.5 Executing AU programs

Once an AU program has been installed, there are 3 different ways to execute it:

1. Enter the name of the AU program. This will work if:

- The AU program is already compiled
- No XWIN-NMR command or macro [1] with the same name exist

2. Enter ***xau au-program-name***

If the AU program is not yet compiled, it will first be compiled and then executed. Otherwise, the program is immediately executed.

3. Enter ***xau***

A list of available AU programs will appear. Click on the AU program you want to execute. If it is not yet compiled, it will first be compiled and then executed. Otherwise, the AU program is immediately executed.

1.6 Viewing AU programs

You can view existing AU programs in the following way:

1. View the entire content of one AU program:

a) Enter ***edau***

A list of all existing AU programs are displayed in two columns. The left column shows the user defined AU programs, the right column the Bruker library AU programs.

b) Click on an AU program in the list

When you select a Bruker AU program, it is shown in *view* mode which means you cannot edit it. When you click on a user-defined AU program it is shown in *edit* mode which means you can change it.

2. Enter ***listall_au***

A list and a short description of all library AU programs is stored in the file `listall` in the users home directory. Note that this list is also available in

1. Here we refer to an XWIN-NMR macro created with ***edmac***

Chapter 12 of this manual.

1.7 About AU macros

We will use the word *macro* rather often throughout this manual referring to AU macros. This should not be confused with XWIN-NMR macros which are files containing a sequence of XWIN-NMR commands. XWIN-NMR macros are created with ***edmac*** and executed with ***xmac***. An AU macro, however, is a statement in an AU program which defines one or more XWIN-NMR commands, library functions or C-language statements. In its simplest form, an AU macro defines one XWIN-NMR command. For example the macros ZG and FT execute the XWIN-NMR commands ***zg*** and ***ft***, respectively. Other macros like FETCHPAR and IEXPNO do not define XWIN-NMR commands, their function is only relevant in the context of an AU program. More complex macros may contain several XWIN-NMR commands and/or C-statements. All macros in AU programs should be written in capital letters. They are automatically translated to the corresponding C-code when the AU program is compiled. AU macros are defined in the file:

```
/xwhome/prog/include/aucmd.h
```

1.8 About Bruker library functions

Bruker library functions are C-functions which are contained in Bruker libraries. They offer several features which are also used in the XWIN-NMR interface, for example the display of a list of datasets from which the user can select one dataset. If you use a Bruker library function in an AU program the corresponding library is automatically linked to the AU program during compilation. The most important and versatile Bruker library functions are described in chapter 9.

1.9 Creating your own AU programs

1.9.1 Writing a simple AU program

Before you start writing an AU program, you might want to check if an AU program already exists which (almost) meets your requirements. If this is not the case, you can write your own AU program in the following way:

1. Enter ***edau <au-name>***
   Your preferred XWIN-NMR text editor will be opened [1]
2. Do one of the following:
   - Insert an existing library AU program and modify it to your needs.
   - Write a new AU program using the macros as described in this manual.

   The first macro in an AU program should always be GETCURDATA, the last macro should always be QUIT (or QUITMSG).
3. Save the file and exit from the editor.
4. A dialogue will appear asking you whether you want to compile the AU program, quit without compilation or go back to a listing of all AU programs:
   - Press **Return** to compile the AU program.

1.9.2 Using variables

Since AU programs are C programs you can use C-language variables. Several variables are already predefined for usage in AU programs. In fact, we distinguish three different types of variables: predefined dedicated variables, predefined general variables and user defined variables.

1.9.2.1 Predefined dedicated variables

Predefined dedicated variables have the following properties:

- they do not need to be declared in an AU program
- their declaration is automatically added during compilation
- they are known to the AU main body and to possible subroutines
- they are set implicitly by certain macros, e.g. the variable expno is set by macros like GETCURDATA, DATASET and IEXPNO
- they should not be set explicitly, so do NOT use statements like:

  ```
  expno = 11;
  FETCHPAR("NS", &expno)
  ```

- they can be evaluated in macros or C-statements, e.g.:

1. You can change the XWIN-NMR text editor by entering the command ***setres.***

```
DATASET(name, expno, 2, disk, "guest")
i1=expno+1;
```

- examples of different types of predefined dedicated variables are:
  char-string: name, disk, user, name2
  integer: expno, procno, loopcount1, loopcount2, lastparflag

A complete list of all predefined dedicated variables with their types can be found in Chapter 1.11.2

1.9.2.2 Predefined general variables

Predefined general variables have the following properties:

- they do not need to be declared in an AU program
- their declaration is automatically added during compilation
- they are known to the AU main body but not to possible subroutines
- they can be freely used for various purposes
- examples of different types of predefined general variables are:
  integer: i1, i2, i3
  float: f1, f2, f3
  double:d1, d2, d3
  char-string: text

A complete list of all predefined general variables with their types and initial values can be found in Chapter 1.11.3.

1.9.2.3 User defined variables

For simple AU programs the number of predefined general variables is sufficient, you do not need to declare any additional variables. For more complex AU programs you might need more variables or you might want to use specific names. In these cases you can define your own variables in the AU program. User defined variables have the following properties:

- they must be declared at the beginning of an AU program
- they can be freely used for various purposes
- they are known to the main AU program but not to possible subroutines
- examples of declarations are:

```
int ivar1, ivar2;
float fvar1, fvar2, fvar3;
double dvar1, dvar2, dvar3;
char cstr1[20], cstr2[200];
```

1.9.3 Using AU macros with arguments

Several AU macros take one or more arguments. Arguments can be constants (values) or variables. In fact, an argument can be specified in four different ways as described here for the macro REXPNO:

- as a constant, e.g.:

  ```
  REXPNO(3)
  ```

- as a predefined dedicated variable e.g.:

  ```
  REXPNO(expno+1)
  ```

- as predefined general variable, e.g.:

  ```
  i1=6;
  REXPNO(i1)
  ```

- as a user defined variable,e.g.:

  ```
  int my_exp;
  ....
  my_exp=1;
  REXPNO(my_exp)
  ```

It is very important that the arguments are of the correct type. Macros can take arguments of the type integer (like REXPNO), float, double or character-string.

Some macros, for example STOREPAR, take XWIN-NMR parameters as arguments and each parameter is of a certain type. For example, the AU statement

```
STOREPAR("O1", d1)
```

stores the value of the variable d1 into the parameter O1. The predefined (double) variable d1 is used since O1 is of the type double. The second argument could also be a constant, e.g.:

```
STOREPAR("O1", 287.15)
```

A list of all XWIN-NMR parameters and their type can be found in Chapter 13.

1.9.4 Using C-language statements

AU programs can contain AU macros but also C-language statements like:

- define statements, e.g.: #define MAXSIZE 32768
- include statements, e.g.: #include <time.h>
- variable declarations, e.g. int ivar;
- variable assignments, e.g.: ivar = 20;
- loop structures, e.g.: for, while, do
- control structures, e.g.: if-else
- C-functions, e.g.: strcpy, strcmp, sprintf

Important: several C-language statements (including declarations of variables) are already predefined and automatically added during compilation of the AU program.

A example of an AU program using macros and C-statements is:

```
int eno, pno;
char datapath [500], dataname[50], datauser[50], datadisk[200];

GETCURDATA
(void) strcpy (dataname,name);
(void) strcpy (datauser,user);
(void) strcpy (datadisk,disk);
eno = expno;
pno = procno;
(void) sprintf (datapath,"%s/data/%s/nmr/%s/%d/pdata/%d/title",
datadisk, datauser, dataname, eno, pno);
if ( (i1 = showfile (datapath)) < 0 )
{
    Proc_err (DEF_ERR_OPT,"Problems with showfile function");
}
QUIT
```

Note that GETCURDATA and QUIT are AU macros, *strcpy* and *sprintf* are C-functions and *showfile* and *Proc_err* are Bruker library functions.

For an explanation of C-functions and more information on C-language we refer to the literature on C-programming.

1.9.5 Additional hints on C-statements

If you are using C-language code in your AU programs, then there are a few things to be considered.

1. Using C-language header files

Several C-language header files are automatically added to your AU program during compilation. If you are using C-code which requires additional header files you must write your AU program in a special way. The main AU program should be a call to a subroutine which performs the actual task of the AU program. The *include* statements for the header file must be entered between the main AU program and the subroutine. This gives the following structure:

```
GETCURDATA
subroutine(curdat, cmd)
QUIT
#include <headerfile.h>

subroutine(curdat,cmd)
char *curdat, *cmd;
{
   MACRO1
   MACRO2
}
```

or

```
subroutine(curdat, cmd)
QUIT
#include <headerfile.h>

subroutine(curdat,cmd)
char *curdat, *cmd;
{

   GETCURDATA
   MACRO1
   MACRO2
}
```

Such a structure is used in several Bruker library AU programs (e.g. amplstab, decon_t1, etc.). Several Bruker library functions like `PrintExpTime`, `gethighest`, `getxwinvers`, `pow_next` and `unlinkpr` also require an in-

clude statement in the AU program (see Chapter 11).

2. Some macros, e.g. IEXPNO and IPROCNO change the current AU dataset but do not make it available for subsequent commands. If they are followed by a CPR_exec or any C-statement which access the current AU dataset, then you must precede that statement with SETCURDATA (see also the descriptions of GETCURDATA, SETCURDATA, IEXPNO etc. in Chapter 4).
3. If you are using C-languages loop statements like *for*, *do* or *while* or control statements like *if*, we strongly recommend to always put the body of such statements between {}. If the body only contains simple macros like ZG or FT you can omit them because these macro definitions already contain {}. However, more complex macros might internally define C-statements that include loop or control structures. If such a macro is used within a loop or control structure in the AU program, then you create nested loops which require the usage of {}.

1.9.6 Viewing Bruker standard AU programs for macro syntax

The syntax of many AU macros is trivial, just enter the XWIN-NMR command in capital letters. Other macros and especially Bruker library functions are more complex. A detailed description of frequently used AU macros and functions can be found in subsequent chapters of this manual. Alternatively, you can also look for an existing AU program containing this macro or function. If, for example, you want to know the syntax of the macro WRPA you can do the following:

On an UNIX workstation:

- open a UNIX shell
- **`cd /<xwhome>/prog/au/src.exam`**
- **`grep -i wrpa *`**

where `<xwhome>` is the directory where XWIN-NMR is installed.

On a Windows PC:

- Click **Start -> Find -> Files or Folders**
- Click **Browse** and open **C:\Bruker\xwin-nmr\prog\au\src.exam**
- Click **Advanced**, in the field **Containing text** enter **`wrpa`**
- Click on **Find now**

assuming XWIN-NMR is installed in `C:\Bruker`.

1.10 How an AU program is translated into C-code

This paragraph is intended for users who want to get a deeper understanding of the compilation process. If you simply want to write and use AU programs you can skip this paragraph.

XWIN-NMR automatically translates your AU program into C-language and compiles it. Files and directories used during AU program compilation are:

```
/<xwhome>/exp/stan/nmr/au/makeau
/<xwhome>/exp/stan/nmr/au/vorspann
/<xwhome>/exp/stan/nmr/au/mk_AUtable.exe
/<xwhome>/prog/include/aucmd.h
/<xwhome>/prog/include/inc
```

The compilation process is entirely controlled by the script `makeau` which performs the following steps.

1. The file `vorspann` is concatenated with your AU program. This file contains a variety of definitions including
   - the C-program *main* statement
   - *#include* statements of C-header files (which in turn contain other definitions)
   - *#define* statements which define constants
   - predefined dedicated variables, e.g.: *name, disk, user, expno, procno*
   - predefined general variables, e.g. : *text, i1, i2, i3, f1, f2, f3, d1, d2, d3*
2. After `vorspann` and your code have been concatenated, a pre-processor program called `mk_AUtable.exe` scans the file for macro definitions and replaces them. The pre-processor searches for macro definitions in the file `aucmd.h` and in the `inc` directory. All AU macros are defined in the ascii file `aucmd.h`. Additional macros are defined in the files in the `inc` directory. In some cases, the name of the macro is the name of one of the files in `inc` directory and the entire content of the file represents that macro.
3. After `mk_AUtable.exe` has generated a C program source file, this file is compiled and an executable program is created. The compilation is done with the GNU C-compiler *gcc*. The linking process is done with the native linker which is part of the native C-compiler *cc*. All AU program's source files reside in:

`/<xwhome>/exp/stan/nmr/au/src`

executables will be stored into:

`/<xwhome>/prog/au/bin`.

The following section shows the result of concatenating `vorspann` with the following AU program:

```
GETCURDATA
EFP
APK
SREF
QUIT
```

For better presentation, only a part of `vorspann` is shown. All variables declared in `vorspann` are listed in chapter 1.10.

```
#include <stdio.h>
#include <stdlib.h>

.....

main(argc,argv)
int argc;
char **argv;
{
char curdat[PATH_MAX];
char arglist[BUFSIZ];
int modret;
modret = AU_program(curdat,arglist);
}

.....

AU_program(curdat,cmd)
char *curdat;
char *cmd;
{
int i1=0,i2=0,i3=0;
float f1=0,f2=0,f3=0,f998=0,f999=0;
double d1=0,d2=0,d3=0;
char text[BUFSIZ/2];
```

GETCURDATA
EFP
APK
SREF
QUIT

Note that the macro QUIT defines the closing C-language '}'statement.

1.11 Listing of all predefined C statements

1.11.1 Including header files

The following C-language header files are automatically included during compilation:

stdio.h, stdlib.h, unistd.h, string.h, errno.h, math.h, limits.h, fcntl.h

which reside in the following directories:

under UNIX : /usr/include
under Windows: C:\Program Files\Microsoft Visual Studio\VC98\Include

and

erropt.h, brukdef.h, lib/uni.h, lib/libcb.h, lib/util.h, sample.h, aucmd.h

which reside in the directory:

/xwhome/prog/include

Note that the latter group of header files is delivered with XWIN-NMR.

1.11.2 Predefined dedicated variables

The following list contains all predefined dedicated variables, their type and the AU macros by which they are set. Note that most variables are set or modified by several macros and only one or two are listed here.

type	variable	set by macros
int	lastparflag	USELASTPARS, USECURPARS
int	loopcount1	TIMES/END
int	loopcount2	TIMES2/END
int	loopcount3	TIMES3/END
int	loopcountinf	TIMESINFINITE
char	disk[256]	GETCURDATA
char	user[64]	GETCURDATA
char	type[16]	GETCURDATA
char	name[64]	GETCURDATA
int	expno	GETCURDATA, IEXPNO
int	procno	GETCURDATA, IPROCNO
char	disk2[256]	GETCURDATA2
char	user2[64]	GETCURDATA2
char	type2[16]	GETCURDATA2
char	name2[64]	GETCURDATA2
int	expno2	GETCURDATA2
int	procno2	GETCURDATA2
char	disk3[256]	GETCURDATA3
char	user3[64]	GETCURDATA3
char	type3[16]	GETCURDATA3
char	name3[64]	GETCURDATA3
int	expno3	GETCURDATA3
int	procno3	GETCURDATA3
char	parsettype[10]	PARSETTYP, SETPARSET
char	namelist[10][64]	SETDATASET
char	dulist[10][256]	SETDATASET

Table 1.1

type	variable	set by macros
char	userlist[10][64]	SETDATASET
char	parsetlist[10][16]	RPARSETLIST
char	pulproglist[10][16]	RPULPROGLIST
int	expnolist[15]	SETDATASET
int	procnolist[15]	SETDATASET
int	loopcountlist[15]	RLOOPCOUNTLIST
float	vtlist[128]	RVTLIST
int	xloopcount	ILOOPCOUNTLIST
int	xpulprog	IPULPROGLIST
int	xparset	IPARSETLIST
int	xdataset	IDATASETLIST
int	xvt	IVTLIST
int	listcount1	TIMESLIST
FILE	*textfilepointer	
FILE	*debug	
char	longpath[PATH_MAX]	
char	Hilfs_string[BUFSIZ/2]	

Table 1.1

1.11.3 Predefined general variables

The following list contains all predefined general variables, their types and initial

values:

type	variable	initial value
int	i1	0
int	i2	0
int	i3	0
double	d1	0
double	d2	0
double	d3	0
float	f1	0
float	f2	0
float	f3	0
float	f998	0
float	f999	0
char	text[BUFSIZ/2]	

Table 1.2

Chapter 2

Inventory of AU macros and Bruker library functions

2.1 Naming conventions

This chapter lists most AU macros and Bruker library functions that are available for AU programming. Simple macros with their short description are only mentioned in this chapter. More complex macros and AU functions are mentioned here and described more extensively in the following chapters. Table 2.1 explains the

macro conventions used in this chapter.

Macro	Explanation
XXX	The macro can be typed "as is". There is no further explanation for the macro in this manual.
XXX(arg1,arg2)	The macro XXX takes two arguments. Because the macro is easy to use, there is no further description in this manual.
XXX *	Like XXX, but there is a detailed description in one of the following chapters.
XXX(....) *	The macro XXX takes one or more arguments and its usage is described in one of the following chapters.

Table 2.1 Macro conventions

Several AU macros that are described in this chapter require one or more arguments. These arguments can be constants or variables as described in Chapter 1.9.3. It is very important to use the correct type of argument in a macro call. The macros described in the tables of this chapter use the following arguments:

integer : i1, i2, i3, eno, pno
float : f1
double : d1
char-string: text, cmd, file, flag, mac, parm, parset, prog, shim, typ, dsk, usr, nam

Note that the arguments *i1*, *i2*, *i3*, *f1*, *d1* and *text* have the same names as the corresponding predefined general variables. The predefined general variables are easy to use because they do not need to be declared. You can, however, use your own variables as macro arguments.

2.2 Macros for dataset handling

Macro	Description
GETCURDATA *	The first AU program statement; get the foreground dataset
SETCURDATA *	Make the current AU dataset available for subsequent AU statements
GETDATASET *	Prompt the user to specify a new dataset

Macro	Description
DATASET(....) *	Set the current AU dataset
DATASET2(....) *	Set the 2nd dataset (like the XWIN-NMR command ***edc2***)
DATASET3(....) *	Set the 3rd dataset (like ***edc2***)
GETCURDATA2	Read the 2nd dataset (like ***edc2***)
GETCURDATA3	Read the 3rd dataset (like ***edc2***)
DEXPNO *	Decrease the experiment number by one
IEXPNO *	Increase the experiment number by one
REXPNO(i1) *	Set the experiment number to the value of i1
DPROCNO *	Decrease the processing number by one
IPROCNO *	Increase the processing number by one
RPROCNO(i1) *	Set the processing number to the value of i1
GDATASETLIST	Prompt the user to enter a dataset list filename and read its contents
GLIST	Prompt the user to enter the dataset list filename and read its contents. In addition to the GDATASETLIST macro, GLIST also expects a pulse program and a parameter set name in the dataset list file.
DDATASETLIST	Decrement to the previous entry in the dataset list
IDATASETLIST	Increment to the next entry in the dataset list
RDATASETLIST(i1)	Read the dataset at position i1 of the dataset list and make it the current AU dataset
IFEODATASETLIST	Checks if the end of the dataset list is reached. The answer is true if there is no further entry.
SETDATASET	Set the current AU dataset to the one currently defined by the dataset list
DU(dsk)	Set the disk unit to *dsk*
SETUSER(usr)	Set the user name to the user *usr*
WRA(i1) *	Copy the raw data to the experiment number i1
WRP(i1) *	Copy the processed data to the processing number i1

Macro	Description
WRPA(....) *	Copy the raw and processed data to the specified dataset
VIEWDATA *	Show the current AU program dataset in XWIN-NMR

2.3 Macros prompting the user for input

Macro	Description
GETDOUBLE(text,d1) *	Prompt the user to enter a double value
GETFLOAT(text,f1) *	Prompt the user to enter a float value
GETINT(text,i1) *	Prompt the user to enter an integer value
GETSTRING(text,nam) *	Prompt the user to enter a text string

2.4 Macros handling XWIN-NMR parameters

Macro	Description
GETPROSOL *	Copy the probehead and solvent dependent parameters to the corresponding acquisition parameters
FETCHPAR(parm,&val) *	Get an acquisition, processing or output parameter
FETCHPAR1(parm,&val)	Get an F1 dimension parameter (2D acquisition/processing)
FETCHPAR3(parm,&val)	Get an F1 dimension parameter (3D acquisition/processing)
FETCHPARS(parm,&val) *	Get a status parameter (acquisition and processing)
FETCHPAR1S(parm,&val)	Get an F1 dimension status parameter (2D)
FETCHPAR3S(parm,&val)	Get an F1 dimension status parameter (3D)
STOREPAR(parm,val) *	Store an acquisition, processing or output parameter
STOREPAR1(parm,val)	Store an F1 dimension parameter (2D)
STOREPAR3(parm,val)	Store an F1 dimension parameter (3D)
STOREPARS(parm,val) *	Store a status parameter (acquisition and processing)
STOREPAR1S(parm,val)	Store an F1 dimension status parameter (2D)

Macro	Description
STOREPAR3S(parm,val)	Store an F1 dimension status parameter (3D)
FETCHPARM(parm,&val)	Get a tomography measurement parameter
STOREPARM(parm,val)	Store a tomography measurement parameter
FETCHPLPAR(parm,&val)	Get a plot parameter
STOREPLPAR(parm,val)	Store a plot parameter
FETCHPLWPAR(parm,&val)	Get a white-washed stacked plot parameter
STOREPLWPAR(parm,val)	Store a white-washed stacked plot parameter
FETCHPLXPAR(parm,&val)	Get an expansion plot parameter
STOREPLXPAR(parm,val)	Store an expansion plot parameter
FETCHT1PAR(parm,&val)	Get a T1 parameter
STORET1PAR(parm,val)	Store a T1 parameter
FETCHDOSYPAR(parm,&val)	Get a dosy (***eddosy***) parameter
STOREDOSYPAR(parm,val)	Store a dosy (***eddosy***) parameter
RPAR(parset,typ) *	Read a parameter set to the current dataset
WPAR(parset,typ) *	Write the current dataset parameters to a parameter set
DELPAR(parset)	Delete the parameter set *parset*
GPARSETLIST	Prompt the user to enter the name of the parameter set list and read its contents
DPARSETLIST	Decrement to the previous parameter set name in the parameter set list
IPARSETLIST	Increment to the next parameter set name in the parameter set list
PARSETTYP(typ)	Set the type of parameter file (acqu, proc, outd or plot) to be read by SETPARSET or RPARSETLIST
RPARSETLIST(i1)	Read the parameter set name from position i1 in the parameter set list and then read the parameters from this parameter set

Macro	Description
SETPARSET	Read the parameters from the parameter set name in position i1 of the parameter list
IFEOPARSETLIST	Checks if the end of the parameter set list is reached. The answer is true if there is no further entry.

2.5 Acquisition macros

Macro	Description
ZG	Start acquisition; if raw data already exist, they are overwritten
GO	Continue the acquisition on already existing raw data by adding to them
II	Initialize acquisition interface
RGA	Automatic receiver gain adjustment
MAKE_ZERO_FID	Create an empty FID
DEG90	Determine 90 degree pulse automatically
GPULPROGLIST	Prompt the user to enter the name of a pulse program list file and read its contents
DPULPROGLIST	Decrement to the previous name in the pulse program list
IPULPROGLIST	Increment to the next name in the pulse program list
RPULPROGLIST(i1)	Read the pulse program name in position i1 of the pulse program list and write it to the acquisition parameters
SETPULPROG	Store the current pulse program name from the pulse program list
IFEOPULPROGLIST	Check if the end of the pulse program list is reached. The answer is true if there is no further entry.

2.6 Macros handling the shim unit and the sample changer

Macro	Description
EJ	Eject sample from the magnet
IJ	Insert sample into the magnet
ROT	Turn rotation on (use value RO from acquisition parameters)
ROTOFF	Turn rotation off and wait until rotation was turned off
LOPO	Set the lock parameters (lock power, lock gain, loop filter, loop time and loop gain)
LFILTER(i1)	Set the loop filter to the value of i1
LG	Auto-adjust the lock gain
LGAIN(f1)	Set the loop gain to the value of f1
LO(f1)	Set the lock power to the value of f1
LTIME(f1)	Set the loop time to the value of f1
LOCK	Lock according to the parameters LOCNUC and SOLVENT using the lock parameters from the ***edlock*** table
RSH(file)	Read the shim values from the specified file
SETSH(shim,i1)	Set one shim to the value of i1
WSH(file)	Write the shim values to the specified file
TUNE(file)	Start autoshimming with the specified tune file
TUNESX	Start autoshimming with the tune file defined by the currently defined probehead and solvent
ZSPOIL(i1)	Set value for Z-spoil gradient pulse from BSMS

2.7 Macros handling the temperature unit

Macro	Description
TESET	Set the temperature on the temperature unit to the value of the acquisition parameter TE.
TEGET	Get the temperature from the temperature unit and store it in the acquisition status parameter TE
TE2SET	Set the temperature on the second regulator of the temperature unit to the value of the acquisition parameter TE2.
TE2GET	Get the temperature from the second regulator of the temperature unit and store it in the acquisition status parameter TE2
TEREADY(i1,f1)	After the temperature is set, wait until it is accurate to f1 degrees for at least 10 sec., then wait i1 seconds for stabilization.
TE2READY(i1,f1)	After the second temperature is set, wait until it is accurate to f1 degrees for at least 10 sec., then wait i1 seconds for stabilization.
TEPAR(file)	Read a file with parameter settings for the temperature unit
GVTLIST	Prompt the user to enter the variable temperature list name and read its contents
RVTLIST	Read the contents of the variable temperature list file defined by the acquisition parameter VTLIST.
DVTLIST	Decrement to the previous value in the vtlist
IVTLIST	Increment to the next value in the vtlist
VT	Read and set the temperature according to the current value of the vtlist

2.8 Macros handling the MAS and HPCU unit

Macro	Description
MASE	Eject sample from MAS unit
MASI	Insert sample into MAS unit
MASR	Set spinning rate according to the acquisition parameter MASR

Macro	Description
MASRGET	Get spinning rate from the MAS unit and store it in the status acquisition parameters
MASG(i1)	Start spinning of sample in MAS with at the most i1 retries
MASH	Halt spinning of sample in MAS
GETHPCU	Get (read) the HPCU parameters
SETHPCU	Set the HPCU parameters
RACKPOW	Switch the HPCU rack power on or off (depending on what the parameter POWMOD is set to)

2.9 1D processing macros

Macro	Description
ABS	Automatic baseline correction (creates intrng file !)
ABSD	Automatic baseline correction with DISNMR algorithm (creates intrng file !)
ABSF	Automatic baseline correction between limits ABSF1 and ABSF2
APK	Automatic phase correction
APK0	Zero order automatic phase correction
APK1	First order automatic phase correction
APKF	Automatic phase correction using the spectral region determined by ABSF2 and ABSF1 for the calculation of the phase values.
APKS	Automatic phase correction especially suitable for polymer spectra
BC	Baseline correction of FID (DC correction)
CONVDTA	Convert digitally filtered FID into analogue (conventional) form
EF	Exponential window multiplication + Fourier transform
EFP	Exponential window multiplication + Fourier transform + phase correction using the processing parameters PHC0 and PHC1
EM	Exponential window multiplication of FID
FMC	Fourier Transform + magnitude calculation

Macro	Description
FP	Fourier Transform + phase correction using the processing parameters PHC0 and PHC1
FT	Fourier Transform
GENFID	Create FID from processed data
GF	Gaussian window multiplication + Fourier Transform
GFP	Gaussian window multiplication + Fourier Transform + phase correction using the processing parameters PHC0 and PHC1
GM	Gaussian window multiplication
HT	Hilbert Transform
IFT	Inverse Fourier Transform
MC	Magnitude calculation
PK	Phase correction using the processing parameters PHC0 and PHC1
PS	Power spectrum calculation
QSIN	Squared sine window multiplication
SAB	Spline baseline correction using base_info file
SINM	Sine window multiplication
SINO	Calculate signal to noise ratio
SREF	Automatic spectral referencing using 2Hlock parameters
TM	Trapezoidal window multiplication
TRF	Processing according to the currently defined processing parameters
UWM	user-defined window multiplication

2.10 Peak picking, integration and miscellaneous macros

Macro	Description
PP	Peak picking according to currently set processing parameters
PPH	Like PP, but with a peak histogram along the listing
PPP	Like PP, but the output is written to the file peaklist in the current processing data directory (PROCNO)

Macro	Description
PPJ	Like PP, but store peaks in JCAMP-DX format
LI	List integrals according to the currently defined intrng file. The macro ABS can be used to create an intrng file.
LIPP	List integrals and all peaks in the integral ranges
LIPPF	Like LIPP, but works always on the full spectrum
NMRQUANT(file)	Do quantitative integration with an nmrquant region file
RLUT(file)	Read color look-up table for 2D or 3D datasets
RMISC(typ,file)	Read a file from one of the following list types: base_info, baslpnts, intrng, peaklist or reg
WMISC(typ,file)	Write a base_info, baslpnts, intrng, peaklist or reg file to its lists directory

2.11 Macros for algebraic operations on datasets

Macro	Description
ADD	Add 2nd and 3rd dataset and put the result into the current dataset. The 3rd dataset is multiplied by DC.
ADDC	Add the constant DC to the current dataset
AND	Put logical "and" of 2nd and 3rd dataset into the current dataset
AT	Same as ADD
CMPL	Put the "complement" of the 2nd and 3rd dataset into the current dataset
DIV	Divide 2nd and 3rd dataset and put the result into the current dataset. The 3rd dataset is multiplied by DC.
DT	Calculate the first derivative of the dataset
FILT	Apply a software digital filter to the current dataset
LS	Left shift spectrum or FID by NSP points
MUL	Multiply 2nd and 3rd dataset and put the result into the current dataset. The 3rd dataset is multiplied by DC.
MULC	Multiply the current dataset with DC
NM	Negate current spectrum

Macro	Description
RS	Right shift spectrum or FID by NSP points
RV	Reverse the spectrum
ZF	Zero the spectrum (1r,1i)
ZP	Zero the first NZP points of the spectrum or FID

2.12 Bayes, deconvolution and T1/T2 macros

Macro	Description
BAYX	Execute Bayesian calculation
BAYED	Edit the Bayes parameters
BAYEDX	Edit the Bayes parameters and then run the calculation
LIBAY	List the result of the Bayesian calculation
VIBAY	Display the result of the Bayesian calculation
GDCON	Gaussian deconvolution of the peaks automatically picked according to the currently set processing parameters
LDCON	Lorentzian deconvolution of the peaks automatically picked according to the currently set processing parameters
MDCON	Mixed Gaussian/Lorentzian deconvolution of the peaks in the peaklist file. The peaklist file can be created with the ***ppp*** command and it can be modified using the ***edmisc*** command.
CT1	Calculate the T1 value of the current peak
DAT1	Calculate T1 value for all peaks picked with PD
DAT2	Calculate T2 value for all peaks picked with PD
PD	Pick data points for relaxation analysis
PD0	Pick data points for relaxation analysis at constant peak position
PF	Peak pick points from a series of FIDs in a 2D ser file
PFT2	Peak pick points from a single FID
SIMFIT	Simplex fit; multiple component relaxation analysis of one peak

Macro	Description
SIMFITALL	Simplex fit; multiple component relaxation analysis of all peaks
SIMFITAS-CALL	Simplex fit; multiple component relaxation analysis of all peaks as defined in the file `t1ascii`

2.13 2D processing macros

Macro	Description
ABS1	Baseline correction in F1 dimension
ABS2	Baseline correction in F2 dimension
ABSD1	Baseline correction in F1 dimension using the DISNMR algorithm
ABSD2	Baseline correction in F2 dimension using the DISNMR algorithm
ABSOT1	Trapezoidal baseline correction in F1 dimension using a slightly different algorithm than abst1
ABSOT2	Trapezoidal baseline correction in F2 dimension using a slightly different algorithm than abst2
ABST1	Trapezoidal baseline correction in F1 dimension using the processing parameters ABSF1, ABSF2, SIGF1, SIGF2
ABST2	Trapezoidal baseline correction in F2 dimension using the processing parameters ABSF1, ABSF2, SIGF1, SIGF2
ADD2D	Add the 2nd dataset to the current dataset.
BCM1	Baseline correction of all columns using the coefficients that were obtained with a manual 1D baseline correction
BCM2	Baseline correction of all rows using the coefficients that were obtained with a manual 1D baseline correction
INVSF	Interchange the frequencies of the two dimensions
LEVCALC	Calculate the levels for the contour representation of the 2D matrix
PTILT	Tilt the 2D matrix by an arbitrary angle
PTILT1	Tilt the 2D matrix along its central vertical line
REV1	Reverse the spectrum in F1 dimension
REV2	Reverse the spectrum in F2 dimension

Macro	Description
SUB1	Subtract 1D spectrum in F1 dimension (no change in sign !)
SUB2	Subtract 1D spectrum in F2 dimension (no change in sign !)
SUB1D1	Subtract 1D spectrum in F1 dimension
SUB1D2	Subtract 1D spectrum in F2 dimension
SYM	Symmetrize COSY spectrum
SYMA	Symmetrize phase sensitive COSY spectrum
SYMJ	Symmetrize J-resolved spectrum
TILT	Tilt J-resolved spectrum by an internally calculated angle
XF1	Fourier transform in F1 dimension
XF1P	Phase correction in F1 dimension using the processing parameters PHC0 and PHC1
XF2	Fourier transform in F2 dimension
XF2P	Phase correction in F2 dimension using the processing parameters PHC0 and PHC1
XFB	Fourier transform in both dimensions
XFBP	Phase correction in both dimensions
XF1M	Magnitude calculation in F1 dimension
XF2M	Magnitude calculation in F2 dimension
XFBM	Magnitude calculation in both dimensions
XF1PS	Power spectrum in F1 dimension
XF2PS	Power spectrum in F2 dimension
XFBPS	Power spectrum in both dimensions
XHT1	Hilbert Transform in F1 dimension
XHT2	Hilbert transform in F2 dimension
XIF1	Inverse Fourier transform in F1 dimension
XIF2	Inverse Fourier transform in F2 dimension
XTRF	2D processing according to processing parameter flags (starts always on the raw data !)

Macro	Description
XTRF2	2D processing according to F2 processing parameter flags only (starts always on the raw data !)
XTRFP	2D Processing according to the processing parameter flags
XTRFP1	2D processing according to the F1 processing parameter flags only
XTRFP2	2D processing according to the F2 processing parameter flags only
ZERT1	Zero a region of each column (F1). The region is determined by ABSF1/ABSF2 (first column) and SIGF1/SIGF2 (last column)
ZERT2	Zero a region of each row (F1). The region is determined by ABSF1/ABSF2 (first row) and SIGF1/SIGF2 (last row)
GENSER	Create a 2D series file from the processed data

2.14 Macros reading and writing projections etc.

Macro	Description
F1SUM(i1,i2,pno)	Read sum of columns from i1 to i2 into the 1D processing number pno
F2SUM(i1,i2,pno)	Read sum of rows from i1 to i2 into the 1D processing number pno
F1DISCO(i1,i2,i3,pno)	Read disco projection between i1 and i2 columns with reference row i3 into the 1D processing number pno
F2DISCO(i1,i2,i3,pno)	Read disco projection between i1 and i2 rows with reference column i3 into the 1D processing number pno
F1PROJN(i1,i2,pno)	Read partial negative projection between columns i1 and i2 into the 1D processing number pno
F1PROJP(i1,i2,pno)	Read partial positive projection between columns i1 and i2 into the 1D processing number pno
F2PROJN(i1,i2,pno)	Read partial negative projection between rows i1 and i2 into the 1D processing number pno

Macro	Description
F2PROJP(i1,i2,pno)	Read partial positive projection between rows i1 and i2 into the 1D processing number pno
PROJ	Calculate the projections of the 2D spectrum
RHNP(pno)	Read horizontal (F2) negative projection into the 1D processing number pno
RHPP(pno)	Read horizontal (F2) positive projection into the 1D processing number pno
RSC(i1,pno) *	Read column i1 of 2D into the 1D processing number pno
RSR(i1,pno) *	Read row i1 of 2D into the 1D processing number pno
RVNP(pno) *	Read vertical (F1) negative projection into the 1D processing number pno
RVPP(pno) *	Read vertical (F1) positive projection into the 1D processing number pno
RSER(i1,eno,pno) *	Read row i1 of 2D raw data into the eno and pno
RSER2D(direc, i1,eno, pno) *	Read plane number i1 in direction direc of 3D raw data into the eno and pno
WSC(i1,pno,eno,nam,usr,dsk) *	Write a column back into position i1 of a 2D dataset defined by pno, eno, nam, usr and dsk
WSR(i1,pno,eno,nam,usr,dsk) *	Write a row back into position i1 of a 2D dataset defined by pno, eno, nam, usr and dsk.
WSER(i1,nam,eno,pno,dsk,usr) *	Write an FID back into position i1 of a 2D raw data defined by eno, pno, nam, dsk and usr.
WSERP(i1,nam,eno,pno,dsk,usr) *	Write a processed FID back into position i1 of a 2D raw data defined by eno, pno, nam, dsk and usr.

2.15 3D processing macros

Macro	Description
TF3(flag,dsk)	Fourier transform in F3 dimension. The flag can be "y" or "n" and determines whether the imaginary parts are stored or not. The processed are stored on disk unit dsk.
TF2(flag)	Fourier transform in F2 dimension (flag as in TF3)
TF1(flag)	Fourier transform in F1 dimension (flag as in TF3)
TF3P(flag)	Phase correction in F3 dimension (flag as in TF3)
TF2P(flag)	Phase correction in F2 dimension (flag as in TF3)
TF1P(flag)	Phase correction in F1 dimension (flag as in TF3)
TABS3	Automatic baseline correction in F3 dimension
TABS2	Automatic baseline correction in F2 dimension
TABS1	Automatic baseline correction in F1 dimension
R12(i1,eno,flag,dsk)	Read F1-F2 plane into a new expno (with or without imaginary parts according to flag) on the unit dsk
R13(i1,eno,flag,dsk)	Read F1-F3 plane into a new expno (with or without imaginary parts according to flag) on the disk unit dsk
R23(i1,eno,flag,dsk)	Read F2-F3 plane into a new expno (with or without imaginary parts according to flag) on disk unit dsk

2.16 XWIN-NMR plotting macros

Macro	Description
PLOT	Plot according to current plot parameters (***edg***)
PLOTX	Plot expansions of the integral ranges as defined with ***edgx***
PLOTS	Suspend plot (put plot in queue)
PLOTW	Plot a white washed stack plot as defined with ***edgw***
FLPLOT	Flush all suspended plots

Macro	Description
LOCKPLOTS	Lock plot queue for current AU program. No other plot commands can now interfere with the suspended plots generated in the current AU program.
UNLOCKPLOTS	Unlock the plot queue of the current AU program.
RMPLOT	Remove all suspended plots from queue
GETLIM	Get frequency of leftmost and rightmost peak from a 1D spectrum and adjust the sweep width of the 1D spectrum to the difference + 10%
GETLCOSY	Get frequency of leftmost and rightmost peak from a 1D spectrum and adjust the sweep width of a COSY spectrum to the difference + 10%
GETLXHCO	Get frequency of leftmost and rightmost peak from two 1D spectra and adjust the sweep width of an X-H correlation spectrum to the difference + 10%
GETLJRES	Get frequency of leftmost and rightmost peak from a 1D spectrum and adjust the sweep width of an J-RESolved spectrum to the difference + 10%
GETLINV	Get frequency of leftmost and rightmost peak from a 1D spectrum and adjust the sweep width of an INVerse spectrum to the difference + 10%

2.17 XWIN-PLOT related macros

XWP_LP *	Create a parameter listing for a plot with XWIN-PLOT
XWP_PP *	Create a peak picking listing for a plot with XWIN-PLOT
AUTOPLOT *	Plot the current dataset according to the XWIN-PLOT layout defined by the ***edo*** parameter LAYOUT.

AUTOPLOT_TO_FILE(filename) *	as AUTOPLOT except that the plot is not sent to the printer but store in the post-script file *filename*.
DECLARE_PORTFOLIO *	Initialize the usage of other XWIN-PLOT portfolio AU macros. Must be inserted at the beginning of the AU program.
CREATE_PORTFOLIO(filename) *	Create the XWIN-PLOT portfolio *filenam*e.
ADD_TO_PORTFOLIO(disk, user, name, expno, procno) *	Add the dataset that is specified with the arguments to the portfolio created with CREATE_PORTFOLIO.
ADD_CURDAT_TO_PORTFOLIO *	Add the current dataset to the portfolio created with CREATE_PORTFOLIO
CLOSE_PORTFOLIO *	Close the definition for the portfolio created with CREATE_PORTFOLIO. Must be used before AUTOPLOT_* macros.
AUTOPLOT_WITH_PORTFOLIO *	Plot the dataset(s) defined in the portfolio created with CREATE_PORTFOLIO according to the layout defined by the ***edo*** parameter LAYOUT.
AUTOPLOT_WITH_PORTFOLIO_TO_FILE(filename) *	as AUTOPLOT_WITH_PORTFOLIO except that the plot is not sent to the printer but store in the postscript file *filename*.

2.18 Macros converting datasets from Aspect 2000/3000 and other vendors

Macro	Description
CONV(....) *	Convert Bruker Aspect 2000/3000 datasets to XWIN-NMR format
CONVCP(....) *	Like CONV but with additional backup copy of the original data
FROMJDX(....) *	Convert a JCAMP-DX file to XWIN-NMR data format
TOJDX(....) *	Convert a dataset to JCAMP-DX format

Macro	Description
JCONV(....) *	Convert a Jeol dataset to Bruker XWIN-NMR format
VCONV(....) *	Convert a Varian dataset to Bruker XWIN-NMR format

2.19 Macros to execute other AU programs, XWIN-NMR macros or commands

Macro	Description
CPR_exec(....) *	C-function for executing special XWIN-NMR commands
WAIT_UNTIL(....) *	Hold the AU program until the specified date and time
XAUA	Execute the acquisition AU program stored in AUNM (***eda***). The next line in the AU program is executed after the AU program AUNM has finished.
XAUP	Execute the processing AU program stored in AUNMP (***edp***). The next line in the AU program is immediately executed after the AU program AUNMP has been started.
XAUPW	Execute the processing AU program stored in AUNMP (***edp***). Like XAUP, but now the next line in the AU program is executed after the AU program AUNMP has finished.
XAU(prog)	Execute the AU program prog with the wait option.
XCMD(cmd) *	Execute the XWIN-NMR command for which no dedicated macro exists.
XMAC(mac)	Execute an XWIN-NMR macro mac.

2.20 Bruker library functions

Macro	Description
CalcExpTime() *	Calculate the experiment time for the current experiment
PrintExpTime(....) *	Print the experiment time for the current experiment
check_pwd(usr) *	Prompt the user usr to enter a password
GetNmrSuperUser() *	Get the name of the current XWIN-NMR superuser

Macro	Description
getdir(....) *	Get all file names and/or directory names within a directory
freedir(....) *	Free memory allocated by `getdir`
uxselect(....) *	Display a list from which an entry can be selected by mouse-click
dircp(....) *	Copy a file
dircp_err(i1) *	Return the error message that corresponds to the error return value of a dircp function call
fetchstorpl(....) *	Read or store one or several plot parameters
gethighest(....) *	Return the next highest unused experiment number of a data-set
getstan(....) *	Return the pathname to the user's current experiment direc-tory
getxwinvers(....) *	Return the current version and patchlevel of XWIN-NMR
mkudir(....) *	Create a complete directory path
PathXWinNMR() *	A class of functions which return pathnames to certain XWIN-NMR directories
pow_next(i1) *	Round i1 to the next larger power of two
Proc_err(....) *	Show a message in a window on the XWIN-NMR screen
Show_status(text) *	Show a string in the status line of XWIN-NMR
showfile(file) *	Show the contents of a file in an XWIN-NMR window
ssleep(i1) *	Pause in an AU program for i1 seconds
unlinkpr(....) *	Delete all processed data files (1r, 1i, 2rr, 2ii etc.) of a dataset

2.21 Macros to return from an AU program

Macro	Description
ABORT	Abort the AU program or any of its subroutines with the return value of -1
ERRORABORT	Return from an AU program or any of its subroutines with the value of AUERR if it is less than 0

Macro	Description
QUIT	Return from an AU program with the value of AUERR. QUIT is usually the last statement of the AU program code.
QUITMSG(text)	Print the text message and then return from the AU program with the value of AUERR. This is an alternative to QUIT.
STOP	Stop the AU program with the return value of AUERR.
STOPMSG("text")	Stop the AU program with the return value of AUERR and display the message "text"

Chapter 3

General AU macros

This chapter contains a description of all general AU macros which can be used for various purposes.

CPR_exec

NAME

CPR_exec - C-function for executing special XWIN-NMR commands

SYNTAX

CPR_exec(char *command, int mode);

DESCRIPTION

CPR_exec is a C-library function which can be used for executing XWIN-NMR commands in AU. The first argument of CPR_exec is an XWIN-NMR command, the second argument must be one of the following values:

WAIT_TERM - wait for the command to finish, then start the next command
CONT_EX - start the command and immediately start the next command

Most commands are available as a dedicated macro, like ZG for ***zg*** and FT for ***ft***. If you want to use XWIN-NMR commands for which no dedicated macro exist, e.g. editor commands or commands with special arguments, then you can use the general macro XCMD which takes only one argument, the XWIN-NMR command. Dedicated macros and XCMD internally call CPR_exec with WAIT_TERM. The only reason to use CPR_exec explicitly is to start a command with CONT_EX, i.e. to run commands simultaneously. In summary:

- Use dedicated AU macros whenever you can
- Use XCMD when no dedicated macro is available
- Use CPR_EXEC only when you want to use CONT_EX

NOTES

Dedicated macros and XCMD call SETCURDATA before they do their actual task. This ensures that they operate on the current AU dataset. If you use CPR_exec explicitly, it is recommended to precede it with SETCURDATA. This is not always necessary but hardly ever wrong (see SETCURDATA).

During sample changer automation, processing and plotting commands are started with CONT_EX to allow simultaneous acquisition on the next sample.

EXAMPLE

The following AU program gets the foreground dataset, runs an acquisition, starts the Fourier Transform and immediately continues an acquisition on the next experiment number:

```
GETCURDATA
TIMES(10)
ZG
CPR_exec("ft", CONT_EX);
IEXPNO
END
QUIT
```

SEE ALSO

XCMD - general macro to execute commands for which no dedicated macro exists

SETCURDATA - make the current AU dataset available for subsequent AU statements

XCMD

NAME

XCMD - execute a command for which no dedicated macro exists

SYNTAX

XCMD(char *command)

DESCRIPTION

XCMD is a general macro to execute XWIN-NMR commands for which no dedicated macro exists. For most XWIN-NMR commands a dedicated macro does exist and we strongly recommend to:

Use dedicated macros whenever available

EXAMPLE

The following AU program gets the foreground dataset, opens the acquisition parameter editor (***eda***) and runs an acquisition and Fourier transform:

```
GETCURDATA
XCMD("eda")
ZG
FT
QUIT
```

SEE ALSO

CPR_exec - C-function for executing special XWIN-NMR commands

WAIT_UNTIL

NAME

WAIT_UNTIL - hold the AU program until the specified date and time

SYNTAX

int WAIT_UNTIL(int hour, int minute, int day, int month)

DESCRIPTION

The function WAIT_UNTIL waits in an AU program until the specified date has been reached. The variables are internally converted to seconds. Every sixty seconds, the function checks whether the current date matches with the selected date. This function basically allows to program an event or command to start at a certain date rather than waiting for a certain time until something is executed.

EXAMPLE

Wait in the AU program until the 31st of October, 6 pm, and then continue:

WAIT_UNTIL(18,0,31,10)

SEE ALSO

ssleep - pause in an AU program for a certain number of seconds

Chapter 4

Macros changing the current AU dataset

This chapter contains a description of all AU macros which can be used to change the current AU dataset, i.e. the dataset on which subsequent AU statements operate.

GETCURDATA

NAME

GETCURDATA - the first AU program statement; get the foreground dataset

SYNTAX

GETCURDATA

DESCRIPTION

GETCURDATA should be the first macro in any AU program and should only be used at the beginning of an AU program. GETCURDATA gets the foreground dataset, i.e. the dataset which is visible when the AU program is started. This dataset becomes the current AU dataset. In fact, GETCURDATA sets the predefined data path variables *disk*, *user*, *type*, *name*, *expno* and *procno* which define the pathname of the current dataset. Subsequent macros, like ZG, FT etc. will then work on this dataset. The current AU dataset can be changed within the AU program with macros like DATASET, IEXPNO or IPROCNO.

GETCURDATA defines the current AU dataset but it takes another macro, SETCURDATA, to make this dataset available for subsequent AU statements. For most predefined macros, like ZG and FT, as well as XCMD etc., this is automatic because SETCURDATA is part of the macro definition.

EXAMPLE

The following AU program gets the foreground dataset and runs an acquisition on it:

```
GETCURDATA
ZG
QUIT
```

SEE ALSO

SETCURDATA - make the current AU dataset available for AU commands
DATASET - set the current AU dataset
GETDATASET - prompt the user to specify a new dataset

SETCURDATA

NAME

SETCURDATA - make the current AU dataset available for subsequent AU statements

SYNTAX

SETCURDATA

DESCRIPTION

SETCURDATA makes the current AU dataset, i.e. the dataset defined by the data path variables *disk*, *user*, *type*, *name*, *expno* and *procno*, available for subsequent AU commands. Normally, you do not need to enter SETCURDATA because it is automatically called by macros which operate on datasets before they perform their actual task. Furthermore, the macros DATASET and GETDATASET, which change the current AU dataset, automatically call SETCURDATA after they performed their actual task. In some cases, however, SETCURDATA must be specified explicitly in the AU program. For example, the macros IEXPNO and IPROCNO change the current AU dataset, but do not call SETCURDATA. If they are followed by a CPR_exec or any C-statement which access the current AU dataset, then you must precede that statement with SETCURDATA.

EXAMPLE

This example shows the part of the library AU program *multizg* which calculates the total experiment time of all acquisitions performed by this AU program:

```
int expTime;
static void PrintExpTime();

GETCURDATA
....

expTime = 0;

TIMES(i1)
   SETCURDATA;
   expTime += CalcExpTime() + 4;
```

```
    IEXPNO;
END
DEXPNO;
....
QUIT
```

Note that IEXPNO is followed by SETCURDATA in the next cycle of the loop.

SEE ALSO

GETCURDATA - the first AU program statement; get the foreground dataset
DATASET - set the current AU dataset
IEXPNO - increase the experiment number by one

DATASET

NAME

DATASET - set the current AU dataset

SYNTAX

DATASET(char *name, int expno, int procno, char *disk, char *user)

DESCRIPTION

The macro DATASET sets the current AU dataset. All data path variables *name*, *expno*, *procno*, *disk* and *user* must be specified as arguments. Subsequent AU commands will operate on this dataset.

EXAMPLE

The following AU program first gets the foreground dataset, then selects a new dataset and runs an acquisition:

```
char[20] newname;
GETCURDATA
strcpy(newname, "glycerine");
DATASET(newname, expno, 3, disk, "peter")
ZG
QUIT
```

The data path variables in this example are entered in the following way:

- *expno* and *disk* keep the values which were obtained with GETCURDATA
- *name* gets the value of *newname*, a variable defined in this AU program
- *procno* and *user* get the values *3* and *peter*, respectively, which are entered as constants

SEE ALSO

GETCURDATA - the first AU program statement; get the foreground dataset
GETDATASET - prompt the user to specify a new dataset
DATASET2 - set the second dataset
IEXPNO - increase the experiment number by one

DATASET2/DATASET3

NAME

DATASET2 - set the second AU dataset
DATASET3 - set the third AU dataset

SYNTAX

DATASET2(char *name, int expno, int procno, char *disk, char *user)
DATA /x/xw2.5

cd SET3(char *name, int expno, int procno, char *disk, char *user)

DESCRIPTION

The macro DATASET2 sets the second AU dataset. The current (first) AU dataset is not affected by this macro. DATASET2 is typically used in combination with algebra macros, like ADD or MUL, which operate on the second and third dataset.

EXAMPLE

The following AU program gets the foreground dataset, adds the spectra of the next processing number and the one after that and stores the result into the current dataset:

```
GETCURDATA
DATASET2(name, expno, procno+1, disk, user)
DATASET3(name, expno, procno+2, disk, user)
ADD
QUIT
```

SEE ALSO

GETCURDATA - the first AU program statement; get the foreground dataset
DATASET - set the current AU dataset
GETDATASET - prompt the user to specify a new dataset

GETDATASET

NAME

GETDATASET - prompt the user to specify a new dataset

SYNTAX

GETDATASET

DESCRIPTION

The macro GETDATASET prompts the user to specify a new dataset. A dialogue is opened and the user is requested to enter the data path variables *name*, *expno*, *procno*, *user* and *disk*. Subsequent AU commands will operate on this dataset. GETDATASET can be used anywhere in an AU program but, since it requires user input, should not be used in fully automated sequences.

NOTE

GETDATASET is not used very often. In AU programs, datasets are usually changed without user interaction, e.g. with the macros DATASET, IEXPNO etc.

EXAMPLE

The following AU program gets the foreground dataset, prompts the user to specify a new dataset and then processes this dataset:

```
GETCURDATA
GETDATASET
EFP
QUIT
```

Actually you could begin this AU program with GETDATASET. This is one of the very few examples where you may omit the macro GETCURDATA.

SEE ALSO

GETCURDATA- the first AU program statement; get the foreground dataset
DATASET - set the current AU dataset
IEXPNO - increase the experiment number by one
IPROCNO - increase the processing number by one

IEXPNO

NAME

IEXPNO - increase the experiment number by one

SYNTAX

IEXPNO

DESCRIPTION

The macro IEXPNO increases the experiment number of the current AU dataset by one. In fact, the value of the data path variable *expno* is incremented by one. Subsequent macros will operate on this new *expno*. IEXPNO is typically used in AU programs which run a series of acquisitions on datasets with the same *name* and successive *expnos*.

EXAMPLE

The following AU program gets the foreground dataset and runs acquisitions on eight successive *expnos*:

```
GETCURDATA
TIMES(8)
   ZG
   IEXPNO
END
QUIT
```

NOTE

IEXPNO must be followed by a SETCURDATA if the AU program continues with an explicit CPR_exec or C-statement (see SETCURDATA).

SEE ALSO

DEXPNO - decrease the experiment number by one
REXPNO - set the experiment number to the specified value
IPROCNO - increase the processing number by one
DATASET- set the current AU dataset

DEXPNO

NAME

DEXPNO - decrease the experiment number by one

SYNTAX

DEXPNO

DESCRIPTION

The macro DEXPNO decreases the experiment number of the current AU dataset by one. In fact, the value of the data path variable *expno* is decremented by one. Subsequent macros will operate on this new *expno*. DEXPNO is typically used after a loop which includes an IEXPNO at the end, to revert the effect of the last (unnecessary) IEXPNO.

EXAMPLE

The following AU program gets the foreground dataset, runs acquisitions on eight successive *expnos* and displays the data of the last *expno*:

```
GETCURDATA
TIMES(8)
   ZG
   IEXPNO
END
DEXPNO
VIEWDATA
QUIT
```

Note that DEXPNO must be followed by a SETCURDATA if the AU program continues with an explicit CPR_exec or C-statement (see SETCURDATA).

SEE ALSO

IEXPNO - increase the experiment number by one
REXPNO - set the experiment number to the specified value
DPROCNO - decrease the processing number by one

REXPNO

NAME

REXPNO - set the experiment number to the specified value

SYNTAX

REXPNO(int number)

DESCRIPTION

The macro REXPNO sets the experiment number of the current AU dataset to the specified value. In fact, the value of the data path variable *expno* is set. Subsequent macros will operate on this new *expno*.

EXAMPLE

The following AU program gets the foreground dataset, runs acquisitions on eight successive *expnos* then sets the current AU dataset back to the first *expno* and Fourier transforms it:

```
GETCURDATA
i1=expno;
TIMES(8)
    ZG
    IEXPNO
END
REXPNO(i1)
FT
QUIT
```

Note that REXPNO must be followed by a SETCURDATA if the AU program continues with an explicit CPR_exec or C-statement (see SETCURDATA).

SEE ALSO

IEXPNO - increase the experiment number by one
DEXPNO - decrease the experiment number by one
RPROCNO - set the processing number to the specified value

IPROCNO

NAME

IPROCNO - increase the processing number by one

SYNTAX

IPROCNO

DESCRIPTION

The macro IPROCNO increases the processing number of the current AU dataset by one. In fact, the value of the data path variable *procno* is incremented by one. Subsequent macros will operate on this new *procno*. IPROCNO is typically used in an AU program which processes a series of datasets with same *name* and *expno* and successive *procnos*.

EXAMPLE

The following AU program runs Fourier transforms on eight successive *procnos*:

```
GETCURDATA
TIMES(8)
   FT
   IPROCNO
END
QUIT
```

Note that IPROCNO must be followed by a SETCURDATA if the AU program continues with an explicit CPR_exec or C-statement (see setcurdata).

SEE ALSO

DPROCNO - decrease the processing number by one
RPROCNO - set the processing number to the specified value
IEXPNO - increase the experiment number by one

DPROCNO

NAME

DPROCNO - decrease the processing number by one

SYNTAX

DPROCNO

DESCRIPTION

The macro DPROCNO decreases the processing number of the current AU dataset by one. In fact, the value of the data path variable *procno* is decremented by one. Subsequent macros will operate on this new *procno*. DPROCNO is typically used after a loop which includes an IPROCNO at the end, to revert the effect of the last (unnecessary) IPROCNO.

EXAMPLE

The following AU program gets the foreground dataset, runs a Fourier transform on eight successive *procnos* and displays the data of the last *procno*:

```
GETCURDATA
TIMES(8)
   FT
   IPROCNO
END
DPROCNO
VIEWDATA
QUIT
```

Note that DPROCNO must be followed by a SETCURDATA if the AU program continues with an explicit CPR_exec or C-statement (see setcurdata).

SEE ALSO

IPROCNO - decrease the experiment number by one
RPROCNO - set the processing number to specified value
DEXPNO - decrease the experiment number by one

RPROCNO

NAME

RPROCNO - set the processing number to the specified value

SYNTAX

RPROCNO(int number)

DESCRIPTION

The macro RPROCNO changes the current AU dataset by setting the processing number to the specified value. In fact, the value of the data path variable *procno* is set. Subsequent macros will then operate on this new *procno*.

EXAMPLE

The following AU program gets the foreground dataset and runs a Fourier transform on eight successive *procnos.*Then the current AU dataset is set back to the first *procno* which is then phase corrected:

```
GETCURDATA
i1=procno;
TIMES(8)
   FT
   IPROCNO
END
RPROCNO(i1)
APK
QUIT
```

Note that RPROCNO must be followed by a SETCURDATA if the AU program continues with an explicit CPR_exec or C-statement (see SETCURDATA).

SEE ALSO

IPROCNO - increase the processing number by one
DPROCNO - decrease the processing number by one
REXPNO - set the experiment number to the specified value

VIEWDATA

NAME

VIEWDATA - Show the current AU program dataset in XWIN-NMR

SYNTAX

VIEWDATA

DESCRIPTION

The macro VIEWDATA shows the current AU program dataset in XWIN-NMR. In other words, the current AU dataset becomes the foreground dataset. VIEWDATA is used whenever the current AU dataset is changed within the AU program, i.e. with DATASET, IEXPNO etc. and this dataset must be shown in XWIN-NMR.

EXAMPLE

The following AU program gets the foreground dataset, increases the processing number and performs a Fourier transform storing the spectrum in this processing number. The spectrum is then shown in XWIN-NMR:

```
GETCURDATA
IPROCNO
FT
VIEWDATA
QUIT
```

SEE ALSO

GETCURDATA - the first AU program statement; get the foreground dataset
GETDATASET - prompt the user to specify a new dataset
DATASET - set the current AU dataset
IEXPNO - increase the experiment number by one
IPROCNO - increase the processing number by one

Chapter 5

Macros copying datasets

This chapter contains a description of all AU macros which can be used to copy the current AU dataset or parts of it to a new dataset.

WRA

NAME

WRA - copy the raw data to the specified experiment number

SYNTAX

WRA(int expno)

DESCRIPTION

The macro WRA copies the raw data, including the acquisition and processing parameters of the current AU dataset to a new experiment number. It does not copy the processed data.

EXAMPLE

The following AU program gets the foreground dataset and copies the raw data to eight successive experiment numbers, starting with *expno* 11:

```
GETCURDATA
i1=11;
TIMES(8)
    WRA(i1)
    i1++;
END
QUIT
```

SEE ALSO

WRP - copy the processed data to the specified processing number
WRPA - copy the raw and processed data to the specified dataset

WRP

NAME

WRP - copy the processed data to the specified processing number

SYNTAX

WRP(int procno)

DESCRIPTION

The macro WRP copies the processed data, including the processing parameters of the current AU dataset, to the specified processing number.

EXAMPLE

The following AU program gets the foreground dataset and copies the processed data to eight successive processing numbers, starting with *procno* 11:

```
GETCURDATA
i1=11;
TIMES(8)
    WRP(i1)
    i1++;
END
QUIT
```

SEE ALSO

WRA - copy the raw data to the specified experiment number
WRPA - copy the raw and processed data to the specified dataset

WRPA

NAME

WRPA - copy the raw and processed data to the specified dataset

SYNTAX

WRPA(char *name, int expno, int procno, char *disk, char *user)

DESCRIPTION

The macro WRPA copies the raw and processed data of the current AU dataset to the specified dataset. WRPA takes 5 arguments, *name*, *expno*, *procno*, *disk* and *user*, i.e. the data path variables which define the dataset path. You can set one, several, or all of these variables to new values in order to define the destination dataset. You can, for instance, archive your data to an external medium by changing the value of the variable *disk* and leaving the other path variables the same.

EXAMPLE

The following AU program copies the current dataset to the jaz drive which is mounted as `/jaz`:

```
GETCURDATA
WRPA(name, expno, procno, "/jaz", user)
QUIT
```

SEE ALSO

WRA- copy the raw data to the specified experiment number
WRP- copy the processed data to the specified processing number

Chapter 6

Macros handling rows/columns

This chapter contains a description of all AU macros which can be used to read (write) rows or columns from (to) a 2D dataset and AU macros that can be used to read rows or planes from 3D raw data.

RSR

NAME

RSR - read a row from a 2D spectrum and store it as a 1D spectrum

SYNTAX

RSR(int row, int procno)

DESCRIPTION

The macro RSR reads a row from a 2D spectrum and stores it as a 1D spectrum. It can be used in the following ways:

- specified with procno > 0, executed on a 2D dataset
  the specified row is stored under the current dataname, the current expno and the specified procno.
- specified with procno = -1, executed on a 2D dataset
  the specified row is stored under dataset ~TEMP/1/pdata/1
- specified with procno > 0, executed on a 1D dataset
  the specified row is read from a 2D dataset that resides under the current dataname, the current expno and the specified procno.
- specified with procno = -1, executed on a 1D dataset
  the specified row is read from the 2D dataset from which the current 1D dataset was extracted (as defined in the file `used_from`).

EXAMPLE

The following AU program gets a 2D dataset and processes it. Then it reads row 16 and stores that under procno 999:

```
GETCURDATA
DATASET("my_2D_data", 1, 1, "/x", "guest")
XFB
RSR(16, 999)
QUIT
```

SEE ALSO

RSC - read a column from a 2D spectrum and store it as a 1D spectrum

RSC

NAME

RSC - read a column from a 2D spectrum and store it as a 1D spectrum

SYNTAX

RSC(int column, int procno)

DESCRIPTION

The macro RSC reads a column from a 2D spectrum and stores it as a 1D spectrum. It can be used in the following ways:

- specified with procno > 0, executed on a 2D dataset
  the specified column is stored under the current dataname, the current expno and the specified procno.
- specified with procno = -1, executed on a 2D dataset
  the specified column is stored under dataset ~TEMP/1/pdata/1
- specified with procno > 0, executed on a 1D dataset
  the specified column is read from a 2D dataset that resides under the current dataname, the current expno and the specified procno.
- specified with procno = -1, executed on a 1D dataset
  the specified column is read from the 2D dataset from which the current 1D dataset was extracted (as defined in the file `used_from`).

EXAMPLE

The following AU program gets a 2D dataset and processes it in the F2 dimension. Then it reads column 128 and processes the resulting 1D dataset:

```
GETCURDATA
DATASET("my_2D_data", 1, 1, "/x", "guest")
XF2
RSC(128, 10)
RPROCNO(10)
EF
QUIT
```

SEE ALSO

RSR - read a row from a 2D spectrum and store it as a 1D spectrum
WSC - replace a column of a 2D spectrum by a 1D spectrum

WSR

NAME

WSR - replace a row of a 2D spectrum by a 1D spectrum

SYNTAX

WSR(int row, int procno, int expno, char *name, char *user, char *disk)

DESCRIPTION

The macro WSR replaces a row of a 2D spectrum by a 1D spectrum. It can be used in the following ways:

- executed on a 1D dataset
  the specified row of the specified dataset (must 2D data) is replaced by the current 1D data.
- executed on a 2D dataset
  the specified row of the current 2D dataset is replaced by the specified dataset (must be 1D data)

Note that WSR exist in this form in XWIN-NMR 3.1 and newer. In XWIN-NMR 3.0 and older, WSR takes only 5 arguments, the expno cannot be specified.

EXAMPLE

The following AU program gets a 2D dataset, reads row 16, phase corrects this row and writes it back to the 2D data:

```
GETCURDATA
DATASET("my_2D_data", 1, 1, "/x", "guest")
XFB
RSR(16, 999)
RPROCNO(999)
APK
WSR(16, 1, expno, name, user, disk)
QUIT
```

SEE ALSO

WSC - replace a column of a 2D spectrum by a 1D spectrum

RSR - read a row from a 2D spectrum and store it as a 1D spectrum

WSC

NAME

WSC - replace a column of a 2D spectrum by a 1D spectrum

SYNTAX

WSC(int column, int procno, int expno, char *name, char *user, char *disk)

DESCRIPTION

The macro WSC replaces a column of a 2D spectrum by a 1D spectrum. It can be used in the following ways:

- executed on a 1D dataset
  the specified column of the specified dataset (must 2D data) is replaced by the current 1D data.
- executed on a 2D dataset
  the specified column of the current 2D dataset is replaced by the specified dataset (must be 1D data)

Note that WSC exist in this form in XWIN-NMR 3.1 and newer. In XWIN-NMR 3.0 and older, WSC takes only 5 arguments, the expno cannot be specified.

EXAMPLE

The following AU program gets a 2D dataset, reads column 16, phase corrects this column and writes it back to the 2D data:

```
GETCURDATA
DATASET("my_2D_data", 1, 1, "/x", "guest")
RSC(16, 999)
RPROCNO(999)
APK
WSC(16, 1, expno, name, user, disk)
QUIT
```

SEE ALSO

WSR - replace a row of a 2D spectrum by a 1D spectrum
RSC - read a column from a 2D spectrum and store it as a 1D spectrum

RSER

NAME

RSER - read a row from 2D or 3D raw data and store it as a 1D FID

SYNTAX

RSER(int row, int expno, int procno)

DESCRIPTION

The macro RSER reads a row from 2D or 3D raw data and stores it as a 1D fid. It can be used in the following ways:

- specified with expno > 0, executed on a 2D dataset
  the specified row is stored under the current dataname and the specified expno. Processing parameters are stored under procno 1.
- specified with expno = -1, executed on a 2D dataset
  the specified row is stored under dataset ~TEMP/1/pdata/1
- specified with expno > 0, executed on a 1D dataset
  the specified row is read from a 2D raw data that resides under the current dataname and the specified expno. Processing parameters are read from procno 1.
- specified with expno = -1, executed on a 1D dataset
  the specified row is read from the 2D dataset from which the current 1D dataset was extracted (as defined in the file `used_from`).

EXAMPLE

The following AU program splits 2D raw data into single fids that are stored in successive expnos:

```
int td;

GETCURDATA
FETCHPAR1S("TD",&td)
i1=0;
TIMES(td)
   i1 ++;
   RSER(i1,i1+expno,1)
```

```
END
QUITMSG("--- splitser finished ---")
```

Note that this is the AU program ***splitser*** that is delivered with XWIN-NMR.

SEE ALSO

WSER - replace a row of 2D raw data by 1D raw data
RSER2D - read a plane from 3D raw data and store it as 2D raw data
RSR - read a row from a 2D spectrum and store it as a 1D spectrum

WSER

NAME

WSER - replace a row of 2D raw data by 1D raw data

SYNTAX

WSER(int row, char *name, int expno, int procno, char *disk, char *user)

DESCRIPTION

The macro WSER replaces a row of 2D raw data by 1D raw data. It can be used in the following ways:

- executed on a 1D dataset
  the specified row of the specified dataset (must be 2D data) is replaced by the current 1D data.
- executed on a 2D dataset
  the specified row of the current 2D dataset is replaced by the specified dataset (must be 1D data)

EXAMPLE

The following AU program writes a number of 1D fids that are stored under the same data name and incremental expnos to 2D raw data.:

```
int ne, exp1, proc1;
char nm1[20];

GETCURDATA

ne=1; exp1=1; proc1=1;

strcpy(nm1, name);
GETSTRING("Enter name of 1D series: ", nm1)
GETINT("Enter starting EXPNO: ", exp1)
GETINT("Enter starting PROCNO: ", proc1)
GETINT("Enter # of Fids: ", ne)
USECURPARS
TIMES(ne)
   WSER(loopcount1+1, nm1, exp1, proc1, disk, user)
   exp1++;
```

```
END
QUIT
```

Note that this is the AU program ***fidtoser*** that is delivered with XWIN-NMR.

SEE ALSO

RSER - read a row from 2D or 3D raw data and store it as a 1D FID
WSR - replace a row of a 2D spectrum by a 1D spectrum
WSC - replace a column of a 2D spectrum by a 1D spectrum

RSER2D

NAME

RSER2D - read a plane from 3D raw data and store it as 2D pseudo raw data

SYNTAX

RSER2D(char *direction, int plane, int expno, int procno)

DESCRIPTION

The macro RSER2D reads a plane from 3D raw data and stores it as 2D pseudo raw data. The first argument, the plane direction can be "s23" or "s13" for the F2-F3 or F1-F3 direction, respectively. The specified plane is stored under the current data name, the specified expno and the specified procno.

RSER2D only exists in XWIN-NMR 3.1 an newer.

EXAMPLE

The following AU program gets a 3D dataset, reads the F2-F3-plane 64 and stores that under expno 11. It then switches to the output 2D dataset and processes it.

```
GETCURDATA
DATASET("my_3D_data", 1, 1, "/x", "guest")
RSER2D("s23", 64, 11, procno)
REXPNO(11)
XFB
END
QUIT
```

SEE ALSO

RSER - read a row from 2D or 3D raw data and store it as a 1D FID
WSER - replace a row of 2D raw data by 1D raw data

Chapter 7

Macros converting datasets

This chapter contains a description of all AU macros which can be used to convert XWIN-NMR data. This includes the conversion of Bruker Aspect 2000/3000 data, Varian data and Jeol data to XWIN-NMR data format as well as the conversion of XWIN-NMR data to JCAMP-DX.

TOJDX

NAME

TOJDX - convert a dataset to JCAMP-DX format

SYNTAX

TOJDX(char *path, int type, int mode, char *title, char *origin, char *owner)

DESCRIPTION

The macro TOJDX converts the current AU data to standard JCAMP-DX format. It takes 6 arguments:

1. the pathname of the output file, e.g. `/tmp/data1.dx`
2. the output type: enter 0, 1 or 2
   0=FID (default), 1=real spectrum, 2=complex spectrum.
3. the compression mode: enter 0, 1, 2 or 3
   0=FIX, 1=PACKED, 2=SQUEEZED, 3=DIFF/DUP (default)
4. the title as it appears in the output file: enter a character-string
5. the origin as it appears in the output file: enter a character-string
6. the owner as it appears in the output file: enter a character-string

If "*" is entered as an argument, then the default value is used.

In XWIN-NMR 3.1 and newer, TOJDX can convert 1D and 2D data. In older versions, it can only convert 1D data.

EXAMPLE

The following AU program gets the foreground dataset and performs a conversion to JCAMP on 5 successive experiment numbers. The name of the JCAMP file contains the *name* and *expno* of the corresponding XWIN-NMR dataset.

```
GETCURDATA
TIMES(5)
   sprintf(text,"/tmp/%s_%d.dx", name, expno);
   TOJDX(text, 0, 3, "*", "*", "*")
   IEXPNO
END
```

QUIT

SEE ALSO

FROMJDX - convert a JCAMP-DX file to XWIN-NMR data format

FROMJDX

NAME

FROMJDX - convert a JCAMP-DX file to XWIN-NMR data format

SYNTAX

FROMJDX(char *input-file, char *overwrite)

DESCRIPTION

The macro FROMJDX converts a JCAMP-DX file to XWIN-NMR data format. It takes 2 arguments:

1. the pathname of the input file, e.g. `/tmp/data1.dx`
2. the overwrite flag which is either "o" or "n"

In XWIN-NMR 3.1 and newer, FROMJDX can convert 1D and 2D data. In older versions, it can only convert 1D data.

EXAMPLE

The following AU program converts all files with the extension `.dx` in the directory `/tmp` to an XWIN-NMR dataset:

```
char **listfile;
GETCURDATA
i1 = getdir ("/tmp",&listfile,"*.dx");
TIMES(i1)
    sprintf(text, "/tmp/%s", listfile[loopcount1]);
    FROMJDX(text, "o")
END
QUIT
```

SEE ALSO

TOJDX - convert a dataset to JCAMP-DX format
`getdir` - get all file names and/or directory names within a directory

CONV/CONVCP

NAME

CONV - convert Bruker Aspect 2000/3000 datasets to XWIN-NMR format
CONVCP - like CONV but with additional backup copy of the original data

SYNTAX

CONV(char *instrument, char *filename)
CONVCP(char *instrument, char *filename, char *targetdir)

DESCRIPTION

The macro CONV converts Bruker Aspect 2000/3000 datasets to XWIN-NMR data format. Input datasets must be stored in the directory:

/<var>/bruknet/<instrument>/<user>

where <var> can be one of the following:

- <du> the disk unit of the current XWIN-NMR dataset
- specified in the file /usr/local/lib/destination (UNIX only)

CONV takes 2 parameters:

1. the instrument where the dataset was acquired, e.g. *ac250*
2. the name of the dataset. If "*" is specified the next available dataset in the storage directory will be converted.

The macro CONVCP is identical to CONV except that it makes a copy of the original data. Therefore, it takes a third argument; the target directory this copy.

EXAMPLE

This example shows the content of the library AU program ***remproc*** which continuously converts all datasets which are sent from an A3000 computer named *asp*. After conversion it processes each dataset by calling a dataset specific processing AU program with the macro XAUPW:

```
#define STATION "asp"

GETCURDATA
CPR_exec("setdef ackn no",CONT_EX);
```

```
TIMESINFINITE
   CONV(STATION,"*")
   GETCURDATA
   XAUPW
END
QUIT
```

VCONV

NAME

VCONV - convert a Varian dataset to Bruker XWIN-NMR format

SYNTAX

VCONV(char *v-name, char *x-name, int expno, char *disk, char *user)

DESCRIPTION

The macro VCONV converts a Varian dataset to XWIN-NMR data format. It takes 5 parameters:

1. the name of the input Varian dataset
2. the name of the output XWIN-NMR dataset
3. the experiment number of the output XWIN-NMR dataset
4. the disk unit of the output XWIN-NMR dataset
5. the user of the output XWIN-NMR dataset

EXAMPLE

The following AU program converts a Varian dataset to XWIN-NMR format:

```
GETCURDATA
VCONV("pinen_h.fid", "pinen_h", 1, "u", "joe")
QUIT
```

SEE ALSO

JCONV - convert a Jeol dataset to Bruker XWIN-NMR format

JCONV

NAME

JCONV - convert a Jeol dataset to Bruker XWIN-NMR format

SYNTAX

JCONV(char *j-name, char *x-name, int expno, char *disk, char *user)

DESCRIPTION

The macro JCONV converts a Jeol dataset to XWIN-NMR data format. It takes 5 parameters:

1. the name of the input Jeol dataset
2. the name of the output XWIN-NMR dataset
3. the experiment number of the output XWIN-NMR dataset
4. the disk unit of the output XWIN-NMR dataset
5. the user of the output XWIN-NMR dataset

EXAMPLE

The following AU program converts a Jeol dataset to XWIN-NMR format:

```
GETCURDATA
JCONV("gx400h.gxd", "gx400h", 1, "u", "joe")
QUIT
```

SEE ALSO

VCONV - convert a Varian dataset to Bruker XWIN-NMR format

Chapter 8

Macros handling XWIN-NMR parameters

This chapter contains a description of AU macros which can be used to get and store XWIN-NMR parameters. Parameters are subdivided in acquisition, processing, output and plot parameters. Furthermore, they exist in two different forms; as foreground and status parameters. Finally, multi-dimensional datasets have parameter sets for each dimension. Different AU macros are available for getting and storing parameters of all categories, forms or dimensions.

FETCHPAR

NAME

FETCHPAR - get an acquisition, processing or output parameter

SYNTAX

FETCHPAR(parm, &val)

DESCRIPTION

The macro FETCHPAR gets the value of a foreground parameter and stores it into an AU variable. This AU variable can then be used in subsequent AU statements. FETCHPAR allows to get acquisition parameters (***eda***), processing parameters (***edp***) and output parameters (***edo***). It is typically used to check or modify a parameter prior to an acquisition or processing statement.

The macro FETCHPAR takes two arguments:

1. the name of the parameter
2. the AU variable into which the parameter value will be stored

There are two important things to be considered:

1. The type of the AU variable must be the same as the type of the parameter (see Chapter 13).
2. The second argument must be specified as the variable's address, i.e. it must be prepended with the '&' character. This, however, does not count for a text variable since a text variable is already an address.

FETCHPAR works on 1D, 2D or 3D datasets and always gets a parameter of the first dimension (F2 for 1D, F2 for 2D and F3 for 3D).

The handling of the macros FETCHPAR1, FETCHPAR3, FETCHPARM, FETCHPLPAR, FETCHPLWPAR, FETCHPLXPAR, FETCHT1PAR and FETCHDOSYPAR is equivalent to the handling of FETCHPAR.

EXAMPLES

The following AU program gets the value of the processing parameter SI and processes the data 4 times, each time doubling the spectrum size and storing the data in successive processing numbers:

```
GETCURDATA
FETCHPAR("SI", &i1)
TIMES(4)
   EFP
   IPROCNO
   i1 = i1*2;
   STOREPAR("SI", i1)
END
QUIT
```

The following AU statements get the values of the acquisition parameter DW and the processing parameter STSI and stores them in the predefined variables *f1* and *i1*, respectively. Then it gets value of the parameter ABSF1 and stores it in the user defined variable *leftlimit*. Finally, it gets the value of the output parameter CURPLOT and stores it in the predefined variable *text*.

```
float leftlimit;
...
FETCHPAR("DW", &f1)
FETCHPAR("STSI", &i1)
FETCHPAR("ABSF1", &leftlimit)
FETCHPAR("CURPLOT", text)
```

SEE ALSO

FETCHPARS - get a status parameter (acquisition and processing)
STOREPAR - store an acquisition, processing or output parameter

FETCHPARS

NAME

FETCHPARS - get a status parameter (acquisition and processing)

SYNTAX

FETCHPARS(parm, &val)

DESCRIPTION

The macro FETCHPARS gets the value of a status parameter and stores it into an AU variable. This AU variable can then be used in subsequent AU statements. Acquisition status parameters are set by acquisition commands and describe the status of the dataset after acquisition. Note that the status parameters (***dpa***) describe what really happened and that this is sometimes different from what was set up before the acquisition as acquisition parameters (***eda***). For example, the status NS is smaller than originally specified when an acquisition was halted prematurely. Any AU program statement which follows an acquisition command and evaluates acquisition parameters must read status parameters. Therefore, FETCHPARS is typically used after acquisition or processing statements, for example for error or abort conditions (see example below).

The macro FETCHPARS takes two arguments:

1. the name of the parameter
2. the AU variable into which the value is value will be stored

There are two important things to be considered:

1. The type of the AU variable must be the same as the type of the parameter (see Chapter 13).
2. The second argument must be specified as the variable's address, i.e. it must be prepended with the '&' character. This, however, does not count for a text variable since a text variable is already an address.

The handling of the macros FETCHPARS1 and FETCHPARS3 is equivalent to the handling of FETCHPARS.

EXAMPLE

The following AU program performs a series of acquisitions on the same dataset

until a minimum signal/noise is reached. In a loop 8 scans are acquired, Fourier transformed and phase corrected. Then the signal/noise of the spectrum is calculated and compared with the minimum value. If the minimum signal/noise was not reached yet, 8 more scans are accumulated etc. A maximum of 8000 scans is acquired. After the acquisition has been stopped, the total number of actually acquired scans is displayed.

```
GETCURDATA
STOREPAR("NS", 8)
GETFLOAT("Please enter the minimum signal/noise", f1)
ZG
TIMES(1000)
    FT
    APK
    SINO
    FETCHPARS("SINO", f2)
    if (f1 >= f2)
        break;
    GO
END
FETCHPARS("NS", i1)
Proc_err (DEF_ERR_OPT,"Acquisition stopped after %d scans", i1);
QUIT
```

SEE ALSO

FETCHPAR - get an acquisition, processing or output parameter
STOREPARS - store a status parameter (acquisition and processing)

STOREPAR

NAME

STOREPAR - store an acquisition, processing or output parameter

SYNTAX

STOREPAR(parm, val)

DESCRIPTION

The macro STOREPAR stores the value of an AU variable into a parameter. This AU variable can then be used in subsequent AU statements. STOREPAR can be used for acquisition parameters (***eda***), processing parameters (***edp***) and output parameters (***edo***). It is typically used to set parameters prior to an acquisition or processing statement. STOREPAR takes two arguments:

1. the name of the parameter
2. the value to be stored which can specified in two different forms:
   - as a constant
   - as the name of an AU variable

Important: the type of the parameter must be the same as the type of the constant or variable. (see Chapter 13).

NOTES

STOREPAR works on 1D, 2D or 3D datasets and always stores a parameter of the first dimension (F2 for 1D, F2 for 2D and F3 for 3D).

The handling of the macros STOREPAR1, STOREPAR3, STOREPARM, STOREPLPAR, STOREPLWPAR, STOREPLXPAR, STORET1PAR and STOREDOSYPAR is equivalent to the handling of STOREPAR.

EXAMPLE

The following AU program reads a standard parameter set, sets the pulse program and power level, asks the user for the number of scans and sets the plotter. Then a dataset is acquired, processed and plotted according to these parameters.

```
char curplotter[20];
```

```
GETCURDATA
RPAR("PROTON", "all")
STOREPAR("PULPROG", "zg30")
STOREPAR("PL 1", 10.0)
GETINT("Please enter the number of scans:", i1)
STOREPAR("NS", i1)
(void) strcpy(curplotter, "hplj5l");
STOREPAR("CURPLOT", curplotter)
ZG
EFP
PLOT
QUIT
```

SEE ALSO

STOREPARS - store a status parameter (acquisition and processing)
FETCHPAR - get an acquisition, processing or output parameter

STOREPARS

NAME

STOREPARS - store a status parameter (acquisition and processing)

SYNTAX

STOREPARS(parm, val)

DESCRIPTION

The macro STOREPARS stores the value of an AU variable into a status parameter. This AU variable can then be used in subsequent AU statements. Status parameters are set by an acquisition or processing command and describe the status of the dataset after this acquisition or processing command. If the data are now manipulated by AU statements which do not update the status parameters, these must be set explicitly with STOREPARS. For example, if you add two fid's with ***addfid***, the total number of scans of the resulting dataset is not automatically updated. This must be done explicitly with STOREPARS.

The handling of the macros STOREPAR1S and STOREPAR3S is equivalent to the handling of STOREPARS.

EXAMPLE

The following AU program reads the foreground dataset, adds the fid of the next experiment number and the experiment number after that and stores the result in the foreground dataset. The number of scans of the original fid's are added and stored in the status parameter NS of the resulting dataset.

```
int expno_save;

GETCURDATA
DATASET2(name, expno+1, procno, disk, user)
DATASET3(name, expno+2, procno, disk, user)
expno_save=expno;
IEXPNO
FETCHPARS("NS", &i1)

IEXPNO
FETCHPARS("NS", &i2)
```

```
REXPNO(expno_save)
ADDFID
STOREPARS("NS", i1+i2)
QUIT
```

SEE ALSO

FETCHPARS - get a status parameter (acquisition and processing)
STOREPAR - store an acquisition, processing or output parameter

RPAR

NAME

RPAR - read a parameter set to the current AU dataset

SYNTAX

RPAR(char *parset, char *typ)

DESCRIPTION

The macro RPAR reads a parameter set to the current AU dataset. This can be a standard Bruker parameter set or a user defined parameter set which was stored with WPAR. RPAR takes two arguments:

1. the name of the parameter set
2. the type of parameters which are to be read

The second argument can be:

- *acqu* for acquisition parameters (***eda***)
- *proc* for processing parameters (***edp***)
- *plot* for plot parameters (***edg***)
- *outd* for output parameters (***edo***)
- *all* for acquisition, processing, plot and output parameters

EXAMPLE

The following AU program reads the standard Bruker parameter set PROTON, sets the number of scans to 1024 and runs an acquisition:

```
GETCURDATA
RPAR("PROTON", "all")
STOREPAR("NS", 1024)
ZG
QUIT
```

SEE ALSO

WPAR - write the current dataset parameters to a parameter set

WPAR

NAME

WPAR - write the current dataset parameters to a parameter set

SYNTAX

WPAR(char *parset, char *typ)

DESCRIPTION

The macro WPAR writes the parameters of the current AU dataset to a parameter set. You can only write to user defined parameter sets. Bruker standard parameters sets cannot be overwritten. WPAR is typically used in AU programs to store a temporary parameter set. It takes two arguments:

1. the name of the parameter set
2. the type of parameters which are to be stored

The second argument can be:

- *acqu* for acquisition parameters (***eda***)
- *proc* for processing parameters (***edp***)
- *plot* for plot parameters (***edg***)
- *outd* for output parameters (***edo***)
- *all* for acquisition, processing, plot and output parameters

EXAMPLE

The following AU program reads the acquisition parameters of the Bruker standard parameter set PROTON, sets the number of scans, the frequency offset and time domain data size and writes the acquisition parameters to a temporary parameter set. It then performs 8 successive acquisitions with these parameters.

```
GETCURDATA
RPAR("PROTON", "all")
STOREPAR("NS", 16)
STOREPAR("O1", 766.23)
STOREPAR("TD",8192)
WPAR("partemp", "acqu")
```

```
TIMES(8)
   ZG
   IEXPNO
   RPAR("partemp", "acqu")
END
QUIT
```

SEE ALSO

RPAR - read a parameter set to the current AU dataset

Chapter 9

Macros for XWIN-PLOT/autoplot

This chapter contains a description of AU macros which can be used to plot data using XWIN-PLOT portfolios and layouts. These include macros for the creation and definition of portfolios and for plotting to the printer, to a postscript file or enhanced metafile.

AUTOPLOT

NAME

AUTOPLOT - plot the current dataset according an XWIN-PLOT layout

SYNTAX

AUTOPLOT

DESCRIPTION

The macro AUTOPLOT plots the current dataset according to the XWIN-PLOT layout that is defined by the ***edo*** parameter LAYOUT.

The XWIN-PLOT layout can be:

- a standard layout that was delivered with XWIN-NMR
- a user defined layout that was setup and stored from XWIN-PLOT

In XWIN-NMR 3.1 and newer, standard processing AU programs, like ***proc_1d*** contain the AUTOPLOT macro for plotting (see the example below) whereas in older versions, the PLOT macro was used. However, AU programs that contain PLOTX macros; are still used in the original form. Furthermore, the old AU programs, using PLOT macro, are still available under the names ***p_**.

EXAMPLE

This AU program processes the current 1D dataset and plots it according to the XWIN-PLOT layout specified in ***edo***:

```
GETCURDATA
EF
APK
SREF
ABS
AUTOPLOT

QUIT
```

SEE ALSO

AUTOPLOT_TO_FILE, AUTOPLOT_WITH_PORTFOLIO, AUTOPLOT_WITH_PORTFOLIO_TO_FILE

AUTOPLOT_TO_FILE

NAME

AUTOPLOT_TO_FILE - as AUTOPLOT but store the output into a file

SYNTAX

AUTOPLOT_TO_FILE(filename)

DESCRIPTION

The macro AUTOPLOT_TO_FILE plots the current dataset according to the XWIN-PLOT layout defined by the ***edo*** parameter LAYOUT. The output is not sent to the printer but stored in the file that is specified as an argument. The argument is normally a full pathname. If it is not, the file is stored in the XWIN-NMR home directory.

If the filename has the extension `.ps`, the output is stored as a postscript file. If (under Windows) it has the extension `.emf`, as in the example below, the output will be stored as an enhanced metafile.

AUTOPLOT_TO_FILE is actually a composite macro that consists of several PORTFOLIO*/AUTOPLOT* macros. This, however, is transparent to the user.

EXAMPLE

This AU program processes the current 1D dataset and plots it according to the XWIN-PLOT layout specified in ***edo***. The result is stored in an enhanced metafile.

```
GETCURDATA

EF
APK
SREF
ABS
AUTOPLOT_TO_FILE("/users/guest/mydata.emf")

QUIT
```

SEE ALSO

AUTOPLOT, AUTOPLOT_WITH_PORTFOLIO

DECLARE_PORTFOLIO

NAME

DECLARE_PORTFOLIO - initialize the use of XWIN-PLOT portfolio macros

SYNTAX

DECLARE_PORTFOLIO

DESCRIPTION

The macro DECLARE_PORTFOLIO initializes the use of other XWIN-PLOT portfolio AU macros. It must be inserted at the beginning of the AU program (before GETCURDATA). Note that this macro initializes portfolio use but does not create one.

EXAMPLE

This AU program plots the current dataset according to the XWIN-PLOT layout specified in ***edo***. It just is a simple demonstration of the use of PORTFOLIO macros.

```
DECLARE_PORTFOLIO

GETCURDATA

CREATE_PORTFOLIO("/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIO
CLOSE_PORTFOLIO

AUTOPLOT_WITH_PORTFOLIO

QUIT
```

Note that this AU program does the same as the command ***autoplot***.

SEE ALSO

CREATE_PORTFOLIO, ADD_TO_PORTFOLIO, CLOSE_PORTFOLIO

CREATE_PORTFOLIO

NAME

CREATE_PORTFOLIO - create a XWIN-PLOT portfolio

SYNTAX

CREATE_PORTFOLIO(name)

DESCRIPTION

The macro CREATE_PORTFOLIO creates the XWIN-PLOT portfolio that is specified as an argument. It takes one argument; the filename of the portfolio.

The argument is normally specified as a full pathname. If it is not, the portfolio is stored under the XWIN-NMR home directory. If the specified file already exists, it is overwritten. Note that CREATE_PORTFOLIO creates the portfolio but does not insert any dataset specifications.

EXAMPLE

This AU program plots the current dataset according to the XWIN-PLOT layout specified in ***edo***. It is just a simple demonstration of the use of PORTFOLIO macros.

```
DECLARE_PORTFOLIO

GETCURDATA

CREATE_PORTFOLIO("/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIO
CLOSE_PORTFOLIO

AUTOPLOT_WITH_PORTFOLIO

QUIT
```

Note that this AU program does the same as the command ***autoplot***.

SEE ALSO

DECLARE_PORTFOLIO, ADD_TO_PORTFOLIO, CLOSE_PORTFOLIO

ADD_CURDAT_TO_PORTFOLIO

NAME

ADD_CURDAT_TO_PORTFOLIO - add the current dataset to the portfolio

SYNTAX

ADD_CURDAT_TO_PORTFOLIO

DESCRIPTION

The macro ADD_CURDAT_TO_PORTFOLIO adds the current dataset to the XWIN-PLOT portfolio that was previously create with CREATE_PORTFOLIO.

EXAMPLE

This AU program plots two datasets, the current and next processing number of the current data name, according to the XWIN-PLOT layout specified in ***edo***.

```
DECLARE_PORTFOLIO

GETCURDATA

CREATE_PORTFOLIO("/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIO
IPROCNO
ADD_CURDAT_TO_PORTFOLIO
CLOSE_PORTFOLIO

AUTOPLOT_WITH_PORTFOLIO
QUIT
```

SEE ALSO

DECLARE_PORTFOLIO, CREATE_PORTFOLIO, CLOSEPORTFOLIO

ADD_TO_PORTFOLIO

NAME

ADD_TO_PORTFOLIO - add the specified dataset to the portfolio

SYNTAX

ADD_TO_PORTFOLIO(disk,user, name, expno, procno)

DESCRIPTION

The macro ADD_TO_PORTFOLIO adds a dataset to the portfolio that was previously created with CREATE_PORTFOLIO. The dataset to be added is completely specified by the five arguments of ADD_TO_PORTFOLIO. Note that these arguments can be constants (values) or variables.

EXAMPLE

This AU program plot two datasets according to the XWIN-PLOT layout specified in ***edo***. Note that the first dataset to be plotted is the so called second dataset (***edc2***), specified by the predefined dedicated variables disk2, user2 etc.

```
DECLARE_PORTFOLIO

GETCURDATA

CREATE_PORTFOLIO(“/temp/myPortfolio.por”)
ADD_TO_PORTFOLIO(disk2, user2, name2, expno2, procno2)
ADD_TO_PORTFOLIO("C:/xw", "guest", "mydata", 1, 3)
CLOSE_PORTFOLIO

AUTOPLOT_WITH_PORTFOLIO

QUIT
```

SEE ALSO

ADD_CURDAT_TO_PORTFOLIO

CLOSE_PORTFOLIO

NAME

CLOSE_PORTFOLIO - closes the portfolio definition

SYNTAX

CLOSE_PORTFOLIO

DESCRIPTION

The macro CLOSE_PORTFOLIO closes the definition of the portfolio that was previously created with CREATE_PORTFOLIO. It must be used after the last ADD_CURDAT_TO_PORTFOLIO or ADD_TO_PORTFOLIO macro and before the first AUTOPLOT* macro.

EXAMPLE

This AU program plots the current dataset according to the XWIN-PLOT layout specified in ***edo***. It is just a simple demonstration of the use of PORTFOLIO macros.

```
DECLARE_PORTFOLIO

GETCURDATA

CREATE_PORTFOLIO("/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIO
CLOSE_PORTFOLIO

AUTOPLOT_WITH_PORTFOLIO

QUIT
```

Note that this AU program does the same as the command ***autoplot***.

SEE ALSO

DECLARE_PORTFOLIO, CREATE_PORTFOLIO, ADD_TO_PORTFOLIO

AUTOPLOT_WITH_PORTFOLIO

NAME

AUTOPLOT_WITH_PORTFOLIO - plot the dataset(s) of the current portfolio

SYNTAX

AUTOPLOT_WITH_PORTFOLIO

DESCRIPTION

The macro AUTOPLOT_WITH_PORTFOLIO plots the dataset(s) defined in the portfolio created with CREATE_PORTFOLIO according to the XWIN-PLOT layout defined by the ***edo*** parameter LAYOUT.

EXAMPLE

This AU program plots the current dataset according to the XWIN-PLOT layout specified in ***edo***. It is just a simple demonstration of the use of PORTFOLIO macros.

```
DECLARE_PORTFOLIO

GETCURDATA

CREATE_PORTFOLIO("/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIO
CLOSE_PORTFOLIO

AUTOPLOT_WITH_PORTFOLIO

QUIT
```

Note that this AU program does the same as the command ***autoplot***.

SEE ALSO

AUTOPLOT, AUTOPLOT_WITH_PORTFOLIO_TO_FILE

AUTOPLOT_WITH_PORTFOLIO_TO_FILE

NAME

AUTOPLOT_WITH_PORTFOLIO_TO_FILE - plot the dataset(s) of the current portfolio and store the output into a file

SYNTAX

AUTOPLOT_WITH_PORTFOLIO_TO_FILE(filename)

DESCRIPTION

The macro AUTOPLOT_WITH_PORTFOLIO_TO_FILE plots the dataset(s) defined in the XWIN-PLOT portfolio that was previously created with CREATE_PORTFOLIO. The plot is made according to the layout defined by the ***edo*** parameter LAYOUT. The output is stored in the file that is specified as an argument to the macro. The argument is normally a full pathname. If it is not, the portfolio is stored under the XWIN-NMR home directory.

If the filename has the extension `.ps`, as in the example below, the output will be stored as a postscript file. If (under Windows) it has the extension `.emf`, the output is stored as an enhanced metafile.

EXAMPLE

This AU program plots the current dataset according to the XWIN-PLOT layout specified in ***edo*** and stores the result into a postscript file.

```
DECLARE_PORTFOLIO

GETCURDATA

CREATE_PORTFOLIO("/temp/myPortfolio.por")
ADD_CURDAT_TO_PORTFOLIO
CLOSE_PORTFOLIO

AUTOPLOT_WITH_PORTFOLIO_TO_FILE("/users/guest/mydata.ps")

QUIT
```

SEE ALSO AUTO

PLOT_WITH_PORTFOLIO, AUTOPLOT_TO_FILE

Chapter 10

Macros prompting the user for input.

This chapter contains a description of all AU macros which can be used to prompt the user for input and store the input into an AU variable. Different macros are available for requesting integer, float, double or text values.

GETINT

NAME

GETINT - prompt the user to enter an integer value

SYNTAX

GETINT("Please enter an integer value : ", i1)

DESCRIPTION

The macro GETINT prompts the user to enter an integer value and stores this value into an integer variable. It can be used for various purposes, for example to set the value of an XWIN-NMR (integer) parameter or to specify the number of cycles in an AU program loop. GETINT takes two arguments:

1. a text string which prompts the user to enter an integer value
2. an integer variable into which the value is stored

EXAMPLE

The following AU program prompts the user for the number of scans per acquisition and the number of experiments to be done:

```
GETCURDATA
GETINT("Please enter the number of scans:", i1)
GETINT("Please enter the number of experiments:", i2)
TIMES(i2)
   STOREPAR("NS", i1)
   ZG
   IEXPNO
END
QUIT
```

SEE ALSO

GETFLOAT - prompt the user to enter a float value
GETDOUBLE - prompt the user to enter a double value
GETSTRING - prompt the user to enter a text string

GETFLOAT/GETDOUBLE

NAME

GETFLOAT - prompt the user to enter a float value
GETDOUBLE - prompt the user to enter a double value

SYNTAX

GETFLOAT(text, f1)
GETDOUBLE(text, d1)

DESCRIPTION

The macro GETFLOAT prompts the user to enter a float value and stores this value into a float AU variable. It is used to get the value for an XWIN-NMR (float) parameter which can then be stored with STOREPAR. GETFLOAT takes 2 arguments:

1. a text string which prompts the user to enter an float value
2. the float variable into which the value is store

The description for GETDOUBLE is equivalent, except that it is used for XWIN-NMR (double) parameters.

EXAMPLE

The following AU program prompts the user for the *frequency offset* and *Gaussian broadening*, stores these values into the parameters O1 and GB respectively and then runs an acquisition, Gaussian multiplication and Fourier transform:

```
GETCURDATA
GETDOUBLE("Please enter the frequency offset:", d1)
STOREPAR("o1", d1);
GETFLOAT("Please enter the Gaussian broadening:", f1)
STOREPAR("GB", f1)
ZG
GM
FT
QUIT
```

SEE ALSO

GETINT - prompt the user to enter an integer value
GETSTRING - prompt the user to enter a text string

GETSTRING

NAME

GETSTRING - prompt the user to enter a text string

SYNTAX

GETSTRING(text, cval)

DESCRIPTION

The macro GETSTRING prompts the user to enter a text string which is then stored into an AU variable. It can be used for various purposes, for example to ask the user a question or prompt the user to enter a name. GETINT takes two arguments:

1. a text string which prompts the user to enter a text string
2. the character-string variable into which the value is stored

EXAMPLE

The following AU program asks the user if an integration must be done and, if yes, which intrng file must be used. Then the integrals are calculated and listed:

```
char answer[8];

GETCURDATA
GETSTRING("Do you want to do an integration (yes/no)?", answer)
if ( !strcmp(answer,"yes") )
{
    GETSTRING("Which intrng file must be used?", text)
    RMISC("intrng", text)
    LI
}
QUIT
```

SEE ALSO

GETINT - prompt the user to enter an integer value
GETFLOAT - prompt the user to enter a float value
GETDOUBLE - prompt the user to enter a double value

Chapter 11

Bruker library functions

This chapter contains a description of various C functions which are available as part of Bruker libraries. Several of them concern the handling of dataset lists or directory lists. You can, for instance, get a list of filenames, display it, select a file from the list and then copy the file to a different directory. The functions described in this chapter are particularly useful for files located in the directories /<xwhome>/conf and /<xwhome>/exp. For copying datasets, we recommend to use the macros described in Chapter 4.

CalcExpTime/PrintExpTime

NAME

`CalcExpTime` - calculate the experiment time for the current experiment
`PrintExpTime` - print the experiment time for the current experiment

SYNTAX

static void PrintExpTime();

int `CalcExpTime` ();
void `PrintExpTime` (int exptime, int expno);

#include<inc/exptutil>

DESCRIPTION

The function `CalcExpTime` calculates the experiment time for the current experiment. The return value is the experiment time in seconds. The function `PrintExpTime` can be used to print the experiment time in the form "days hours minutes seconds".

EXAMPLE

The following AU program calculates and prints the experiment time of a sequence of 10 experiments starting with the foreground dataset.

```
static void PrintExpTime();

GETCURDATA
TIMES(10)
   PrintExpTime(CalcExpTime(),loopcount1);
   IEXPNO
END
QUIT
#include<inc/exptutil>
```

Note that the declaration of `PrintExpTime` must appear at the beginning of the AU program and the #include statement at the end of the AU program.

SEE ALSO

`multiexpt` - a standard Bruker library AU program

check_pwd, GetNmrSuperUser

NAME

`check_pwd` - prompt the user to enter a password
`GetNmrSuperUser` - get the name of the XWIN-NMR NMR superuser

SYNTAX

int `check_pwd` (char *username);
`char *GetNmrSuperUser();`

DESCRIPTION

The function `check_pwd` prompts the user for the password of the specified user. The return value is 0, if the correct password was entered. In all other cases, the return value is -1. This function can be combined with the function `GetNmrSuperUser` which returns the name of the XWIN-NMR NMR superuser.

EXAMPLE

```
GETCURDATA
if ( check_pwd (GetNmrSuperUser()) != 0)
{
    Proc_err(DEF_ERR_OPT,"Sorry, you are not privileged");
    ABORT
}
else
{
    Proc_err(DEF_ERR_OPT,"OK, you may proceed !");
}
QUIT
```

getdir

NAME

`getdir` - get all file names and/or directory names within a directory

SYNTAX

int `getdir` (char *directory, char ***filelist, char *match-code);

DESCRIPTION

The function `getdir` opens a directory and gets all file and directory names in that directory. This list is stored in a 2 dimensional character-string variable which can be evaluated by subsequent AU statements. The list can be limited by specifying a match-code; only names matching this string are entered into the list. `getdir` takes three arguments:

1. the source directory
2. the variable into which the list of names is stored
3. the match-code; an arbitrary string of characters

The third argument, can also be "/files" to get all files but not directories, or "/dir" to get all directories but not files.

The return value of `getdir` is the number of successfully matched file names and/or directory names.

The function `getdir` is frequently used in connection with the `uxselect` function which is also described in this chapter. `getdir` internally allocates memory for the list of names. Officially, you must free this memory with the Bruker library function `freedir`. In practice, however, you can omit `freedir` because all memory allocated by the AU program is automatically freed when the AU program finishes.

EXAMPLES

The following AU statements will create a list of experiment directories from an XWIN-NMR dataset. All entries are returned because no match-code was specified.

```
char sourcedir[200], **listfile;
GETCURDATA
```

```
sprintf (sourcedir, "%s/data/%s/%s/%s/",disk,user,type,name);
i1 = getdir (sourcedir,&listfile,NULL);
```

The following AU statements will create a list of shim files starting with the letters a to p from the bsms directory.

```
char sourcedir[200], **listfile;
GETCURDATA
sprintf (sourcedir, "%s/lists/bsms/",getstan(0,0));
i1 = getdir (sourcedir,&listfile,"[a-p]*");
```

The following AU statement will create a list of all files but not directories from the users home directory.

```
i1 = getdir (getenv("HOME"),&listfile,"/files");
```

The following AU statement will return a list of all directory names from the users home directory.

```
i1 = getdir (getenv("HOME"),&listfile,"/dir");
```

SEE ALSO

`uxselect` - display a list from which an entry can be selected by mouse-click
`freedir` - free memory allocated by `getdir`

freedir

NAME

`freedir` - free memory allocated by `getdir`

SYNTAX

void `freedir` (char **listfile);

DESCRIPTION

The function `freedir` frees the memory that was allocated by a `getdir` function call.

EXAMPLE

See the example under the function `uxselect`.

SEE ALSO

`getdir` - get all file names and/or directory names within a directory
`uxselect` - display a list from which an entry can be selected by mouse-click

uxselect

NAME

`uxselect` - display a list from which an entry can be selected by mouse-click

SYNTAX

char *`uxselect` (char *sourcedir, char **listfile, char *headerline, int mode);

DESCRIPTION

The function `uxselect` displays a list of names, like file names or directory names, and allows the user to select of one of these names. Depending on the mode with which `uxselect` was called the entries in the list can be viewed, renamed, deleted, new entries can be added etc.Note that `uxselect` does not create the list of names. Before you use `uxselect` in an AU program, you must first create such a list with another AU statement, e.g. with the function `getdir`.

The function `uxselect` takes four arguments:

1. the directory in which the listed files/directories reside
2. the variable containing the list of names
3. the header line which appears at the top of the selection window
4. the mode which determines the layout and functionality of the selection window

The first argument must be an actual directory name when the fourth argument (mode) is SEL_DIR_SUB, SEL_WR_CONF, SEL_RENAME or SEL_DELETE. Only in those cases, the `uxselect` function needs to know the source directory because it will access it. For all other modes, `uxselect` will simply use the list of names as it was created by a previous AU statement (like getdir) and the first argument of can be NULL.

The return value of `uxselect` is a character-string, usually the selected file or the directory name. The return value can be assigned to a variable and used in subsequent AU statements. If, however, you close the selection window by clicking the ***Cancel*** button the return value of `uxselect` is NULL.

The following modes are available.

- SEL_READ 0

A list of names is displayed in *select* mode. If you select an entry it becomes the return value of `uxselect` and can be used in subsequent AU statements.

- SEL_WRITE 1

  A list of names is displayed in *select* mode. Furthermore, a new name can be entered at the bottom of the screen. If you select an entry or enter a new name, this will be the return value of `uxselect`. Note that entering a new name does not automatically create a file or directory with this name. You can use the return value in subsequent AU statements.

- SEL_DIR_ONLY 2

  A list of names is displayed in *view only* mode. No entry can be selected, but the whole listing can be printed out.

- SEL_DIR_SUB 3

  A list of directory names is displayed in *view only* mode. This mode can only be used for lists of directory names, not file names. All entries in the directories (files and subdirectories) are also displayed.

- SEL_RD_WIDE 4

  A list of names is displayed in *select* mode in an extra wide window. If the user selects an entry, this becomes the return value of `uxselect`. This mode is similar to SEL_READ.

- SEL_WR_CONF 5

  A list of names is displayed in *select* mode. Furthermore, a new name can be entered at the bottom of the screen. If you select an entry or enter a new name, the overwrite permissions of the corresponding file or directory are checked. If it is writable, the name will be the return value of `uxselect`. This mode is used in the XWIN-NMR command ***wpar***. There are hardly any applications for this mode in AU programs.

- SEL_RENAME 6

  A list of names is displayed in *write* mode. Selecting an entry allows to rename it.

- SEL_ED_WIDE 7

  The list of names is displayed in *write* mode. An empty entry is added in which a new name can be entered. Every entry in the list can be renamed. This mode is used in the XWIN-NMR command ***edhead***. There are hardly

any applications for this mode in AU programs.

- SEL_ALL 8

  A list of names is displayed in *select* mode. You can select a single entry or click the button ***Select all*** to select all entries.

- SEL_DELETE 9

  A list of names is displayed in *select* mode. The selection window contains the buttons ***execute*** and ***select all***. When you select an entry and click on ***execute*** the corresponding file or directory is deleted. When you click ***select all*** and then ***execute***, all files/directories in the list are deleted.

We strongly recommend to specify the mode with its symbolic name rather than with its number. The reason is that the numbers might change in future releases of XWIN-NMR, but the symbolic names will not.

EXAMPLE

The following AU program will get a listing of all shim files with the extension `.mike` and will display this list in a selection window. If an entry is selected, then the corresponding shim file is read with the macro RSH. If no entries were found or selected, the AU program aborts.

```
char sourcedir[200], **listfile, *answer;

GETCURDATA
sprintf (sourcedir, "%s/lists/bsms/",getstan(0,0));
if ( (i1 = getdir (sourcedir,&listfile,"*.mike")) <= 0 )
{
    Proc_err (DEF_ERR_OPT,"No shim files with extension .mike found");
    ABORT
}
else
{
     if ( (answer = uxselect(NULL,listfile,"shim files",SEL_READ)) != 0 )
    {
        RSH(answer)
    }
}
freedir (listfile);
QUIT
```

SEE ALSO

`getdir` - get all file names and/or directory names within a directory
`getstan` - return the pathname to the user's current experiment directory

dircp

NAME

`dircp` - copy a file
`dircp_err` - return the error message that corresponds to the error return value of a `dircp` function call

SYNTAX

`dircp` (char *sourcefile, char *targetfile);
char `*dircp_err` (int return-value);

DESCRIPTION

The function `dircp` copies the sourcefile into the targetfile. If the targetfile exists, it will be overwritten. A negative number is returned if copying was not possible. The function `dircp_err` will return the corresponding C error message. A return value of 0 indicates successful execution.

EXAMPLE

The following AU program copies the `title` file of the foreground dataset to the users home directory.

```
char sourcefile[200], targetfile[200];

GETCURDATA
sprintf (sourcefile, "%s/data/%s/%s/%s/%d/pdata/%d/title",
                        disk,user,type,name,expno,procno);
sprintf (targetfile, "%s/title",getenv("HOME"));
if ( (i1 = dircp (sourcefile,targetfile)) < 0 )
    Proc_err (DEF_ERR_OPT, dircp_err(i1));
QUIT
```

fetchstorpl

NAME

`fetchstorpl` - read or store one or several plot parameters

SYNTAX

int `fetchstorpl` (char *directory, int mode, int where, varargs);

DESCRIPTION

The function `fetchstorpl` can read or write one or several plot parameters in one function call. This routine is primarily used when several plot parameters are to be stored. `Fetchstorpl` is also used when plot parameters are to be stored in a parameter set rather than an XWIN-NMR dataset. If you simply want to get or store one plot parameter, you can use the FETCHPLPAR and STOREPLPAR macros, respectively.

`fetchstorpl` takes four arguments:

1. directory
   Must be *curdat* if the third argument (where) is 0
   Must be the pathname to a parameter set if the third argument (where) is 1
2. mode
   Must be 0 if the parameters are to be stored.
   Must be 1 if the parameters are to be read.
3. where
   Must be 0 if the parameters are to be stored in a dataset.
   Must be 1 if the parameters are to be stored in a parameter set.
4. varargs consists of two parts
   - A list of plot parameters separated by white spaces. This list must be double quoted with " " which makes it a character-string.
   - A list of values or variables, all separated by commas. Each value or variable must match the type of parameter from the above mentioned list.

EXAMPLE

- This example stores CX and CY in the parameter set PROTON.AB:
  (void) sprintf (text,"%s/par/PROTON.AB",getstan(0,0));

i1 = fetchstorpl(text,0,1,"CX CY",20.0,12.0);
Note that this will only work, if the parameter set is writable for the user who runs the AU program.

- This example stores CX and CY in the current AU program dataset:
  i1 = fetchstorpl(curdat,0,0,"CX CY",20.0,12.0);
  Note that the variable `curdat` has a special meaning. In any AU program, `curdat` always and automatically refers to the current AU program dataset.
- This example reads SXLLEFT, SHEI, DHEI and CY from the current AU program dataset:
  float sxlleft, shei, dhei, cy;
  i1 = fetchstorpl(curdat,1,0,"SXLLEFT SHEI DHEI CY",
  &sxlleft,&shei,&dhei,&cy);

SEE ALSO

FETCHPLPAR - get a plot parameter
STOREPLPAR - store a plot parameter
stack1d - generate a stacked plot of 1D spectra from a series of experiments

gethighest

NAME

`gethighest` - return the next highest unused experiment number of a dataset

SYNTAX

int `gethighest` (char *directory);

#include <inc/sysutil>

DESCRIPTION

The function `gethighest` scans a directory for all subdirectories whose name is a number and returns then returns the next highest unused number. `gethighest` is typically used to scan a dataset name directory of an XWIN-NMR dataset. In that case, it returns the highest unused experiment number. If, for example, the highest used experiment number is 56, the function will return the value 57. The function can also be used to return the highest unused processing number of a dataset.

EXAMPLE

The following AU program will copy the current XWIN-NMR experiment into the next highest unused experiment dataset.

```
GETCURDATA
(void) sprintf (text,"%s/data/%s/nmr/%s",disk,user,name);
i1 = gethighest (text);
WRA(i1)
QUIT
#include <inc/sysutil>
```

Note that the #include statement must be included at the end of the AU program.

getstan

NAME

`getstan` - return the pathname to the user's current experiment directory

SYNTAX

char *`getstan` (char *pathname, const char *subdir);

DESCRIPTION

The function `getstan` returns the pathname to the user's current experiment directory. The returned pathname can be concatenated with a known subdirectory pathname as a part of the same `getstan` function call.

EXAMPLE

The following AU program will get the pulse program of the current AU dataset. It will then prompt the user to confirm the name of the pulse program or to enter a new name. Finally, the pulse program will be shown in an XWIN-NMR window.

```
char pulprog[80];

GETCURDATA
FETCHPAR("PULPROG",pulprog)
GETSTRING ("Enter the name of the pulse program: ",pulprog);
(void) sprintf (text,"%s/%s",getstan (NULL,"lists/pp"),pulprog);
showfile (text);
QUIT
```

NOTE

In the above example, the function call `getstan` (NULL,"lists/pp") returns the pathname /<xwhome>/exp/stan/nmr/lists/pp. The function call `getstan`(NULL,NULL) returns /<xwhome>/exp/stan/nmr/.

SEE ALSO

`PathXWinNMR` - a class of functions which return pathnames to certain XWIN-NMR directories
`multi_integ` - an AU program for multiple integrations in AI mode.

getxwinvers

NAME

`getxwinvers` - return the current version and patchlevel of XWIN-NMR

SYNTAX

int `getxwinvers` (char *curversion);

#include <inc/sysutil>

DESCRIPTION

The function `getxwinvers` returns the version and patchlevel of the currently running XWIN-NMR program into the variable `curversion`. This variable can then be printed out.

EXAMPLE

The following AU program prints the current version and patchlevel in the status line of XWIN-NMR.

```
char curversion[80];

GETCURDATA
i1 = getxwinvers(curversion);
show_status (curversion);
QUIT
#include <inc/sysutil>
```

Note that the #include statement must be included at the end of the AU program.

mkudir

NAME

`mkudir` - create a complete directory path

SYNTAX

int `mkudir` (char *directory);

DESCRIPTION

The function `mkudir` scans the specified directory for the last /. Then it checks recursively for the existence of all components of the directory path and creates them if necessary. The function returns -1 if an error occurs, otherwise 0.

If the full pathname is to be created, then the directory must end with a / (see the example below).

EXAMPLE

The following AU program will create a dataset which has an experiment number one higher than the current foreground dataset.

```
GETCURDATA
(void) sprintf (text,"%s/data/%s/nmr/%s/%d/pdata/%d/",
                        disk,user,name,expno+1,procno);
if (mkudir(text) < 0)
    Proc_err (DEF_ERR_OPT, "could not create :\n%s",text);
QUIT
```

PathXWinNMR

NAME

`PathXWinNMR` - a class of functions which return pathnames to certain XWIN-NMR directories

SYNTAX

char *`PathXWinNMRConf` ();
char *`PathXWinNMRCurDir` ();
char *`PathXWinNMRDotXWinNMR` ();
char *`PathXWinNMRExp` ();
char *`PathXWinNMRPlot` ();
char *`PathXWinNMRProg` ();

DESCRIPTION

The above functions return pathnames to certain XWIN-NMR mostly subdirectories of the XWIN-NMR directory <xwhome>. For a standard installation, <xwhome> is:

- on UNIX systems: /u
- on Windows systems: C:\Bruker

For a user-defined installation, <xwhome> can be any directory. The following table lists the directory pathnames returned by the above functions. For examples, please check the Bruker AU program library.

char *`PathXWinNMRConf`	: returns /<xwhome>/conf
char *`PathXWinNMRCurDir`	: returns /<xwhome>/prog/curdir
char *`PathXWinNMRDotXWinNMR`	: returns $HOME/.xwinnmr-hostname
char *`PathXWinNMRExp`	: returns /<xwhome>/exp
char *`PathXWinNMRPlot`	: returns /<xwhome>/plot
char *`PathXWinNMRProg`	: returns /<xwhome>/prog

SEE ALSO

`getstan` - return the pathname to the user's current experiment directory

pow_next

NAME

`pow_next` - round to the next larger power of two

SYNTAX

int `pow_next` (int i1);
#include <inc/sysutil>

DESCRIPTION

The function `pow_next` takes i1 and rounds it to the next larger integer value which is a power of two. The return value of the function is this power of two value. The function has no error handling. If i1 is smaller than 1, then the function will return 1.

EXAMPLE

The following AU program will return 8192 in i2 because this is the next larger number (compared to i1) which is a power of two.

```
GETCURDATA
i1 = 7000;
i2 = pow_next(i1);
QUIT
#include <inc/sysutil>
```

Note that the #include statement must be included at the end of the AU program.

Proc_err

NAME

`Proc_err` - show a error message in a window on the XWIN-NMR screen

SYNTAX

int `Proc_err` (int flag, char *format);

int `Proc_err` (int flag, char *format, varargs);

DESCRIPTION

The function `Proc_err` can be used to construct a error message which will be displayed in a window on the XWIN-NMR screen. The function takes two or three arguments:

1. a flag which determines the type and the number (2 or 3) of buttons in the error window.
2. the error message to be displayed. If this argument contains %d, %f, or %s statements, then `Proc_err` needs a third argument which provides the corresponding variables.
3. variables who's values replace the corresponding %d, %f, or %s statements of the second argument.

The first argument (flag) can have the following values:

- DEF_ERR_OPT
  The error window has one button (***OK***). The AU programs holds until the user clicks ***OK***.
- INFO_OPT
  The error window has one button (Seen). The AU program continues but the error window remains on the screen until it is cleared by another error window or the user clicks ***Seen***.
- QUESTION_OPT
  The error window has two buttons, OK and CANCEL. `Proc_err` returns ERR_OK (0) if the ***OK*** button is clicked and ERR_CANCEL (-1) if the ***CANCEL*** button is clicked. The return value is normally used by subsequent control statements to decide whether or not to continue the AU program.

Note that the message in the `Proc_err` window is constructed in the same way as the C function `sprintf` constructs its strings.

EXAMPLE

The following examples show several possibilities of constructing error messages for the `Proc_err` function call.

- Example for DEF_ERR_OPT :
```
(void) sprintf (text,"%s/data/%s/nmr/%s/%d/pdata/%d/",
                        disk,user,name,expno+1,procno);
Proc_err (DEF_ERR_OPT, "could not create :\n%s",text);
```
- Example for QUESTION_OPT :
```
i1 = Proc_err(QUESTION_OPT,"Continue with the AU program ?\n\
Click OK to continue, click cancel stop");
if ( i1 == ERR_OK )
{
    /* Further AU statements */
}
if ( i1 == ERR_CANCEL )
{
 ABORT
}
```
- Example for INFO_OPT :
```
i1 = 7;
i2 = 5;
Proc_err(INFO_OPT,"%d is bigger than %d",i1,i2);
```

SEE ALSO

`Show_status` - show a string in the status line of XWIN-NMR

All AU programs from the Bruker AU program library which use `Proc_err`

Show_status

NAME

`Show_status` - show a string in the XWIN-NMR status line

SYNTAX

void `Show_status` (char *text);

DESCRIPTION

The function `Show_status` displays the specified text in the XWIN-NMR status line. This function can be used as an alternative to the `Proc_err` function. One difference to `Proc_err` is that there is no window that needs to be acknowledged.

EXAMPLE

The following AU program will display the line "The AU program test has started" in the status line of XWIN-NMR:

```
GETCURDATA
(void) strcpy(text,"The AU program test has started");
Show_status (text);
QUIT
```

SEE ALSO

Proc_err - show a message in a window on the XWIN-NMR screen

showfile

NAME

`showfile` - show the contents of a file in an XWIN-NMR window

SYNTAX

int `showfile` (char *file);

DESCRIPTION

The function `showfile` reads the specified file and displays it in an XWIN-NMR window. This display is a read-only display, so the file cannot be changed.

EXAMPLE

The following AU program will show the title file in an XWIN-NMR window.

```
GETCURDATA
(void) sprintf (text,"%s/data/%s/nmr/%s/%d/pdata/%d/title",
disk,user,name,expno,procno);
i1 = showfile (text);
QUIT
```

ssleep

NAME

`ssleep` - pause in an AU program for a certain number of seconds

SYNTAX

int `ssleep` (int seconds);

DESCRIPTION

The function `ssleep` will cause the AU program to wait with the execution of the next statement until the specified number of seconds has elapsed.

EXAMPLE

The following AU program will wait for 3 minutes before it resumes execution.

```
GETCURDATA
i1 = ssleep (180);
EFP
QUIT
```

SEE ALSO

WAIT_UNTIL - hold the AU program until the specified date and time

unlinkpr

NAME

`unlinkpr` - delete all processed data files (1r, 1i, 2rr, 2ii etc.) of a dataset

SYNTAX

int `unlinkpr` (char *directory);

#include <inc/sysutil>

DESCRIPTION

The function `unlinkpr` deletes all processed data files (`1r`, `1i`, `2rr`, `2ii`, `2ri`, `2ir`, `dsp`, `dsp.hdr`, `dsp_low`) in the specified dataset directory. There is no error check whether the files could be deleted; the return value of the function is always 0 and can be ignored.

EXAMPLE

The following AU program will delete the processed data files of the foreground dataset.

```
GETCURDATA
(void) sprintf (text,"%s/data/%s/nmr/%s/%d/pdata/%d",
disk,user,name,expno,procno);
i1 = unlinkpr (text);
QUIT
#include <inc/sysutil>
```

Note that the #include statement must be included at the end of the AU program.

Chapter 12

List of Bruker AU programs

12.1 Short description of all Bruker AU programs

This chapter contains a list with the names and short-descriptions of all Bruker library AU programs. This list was made for XWIN-NMR 3.1. Some AU programs are not available for older versions of XWIN-NMR.

Z-spoil	Set a Z-spoil value within the SCM.
abs2.water	Performs an F2 baseline correction on a 2D dataset left and right of the water peak.
abs2D	Performs a baseline correction on a 2D dataset in both dimensions.
acqu_fid_ser	Acquires a single FID of the current 2D experiment and replaces the old fid in the ser file.
acqulist	Set up and start acquisitions using f1, f2, f3, vt, vc, vd, vp lists.
amplstab	Calculates the amplitude stability based on a peaklist file.
angle	Perform multiple acquisitions and ft's. This program is particularly interesting when you want to adjust the magic angle for MAS type experiments.
asclev	Converts the level file in the current processed data directory to ASCII and writes it to the file
au_getl1d	Acquire sweep width optimized 1D spectra.
au_getlcosy	Acquire sweep width optimized COSY spectra.
au_getlinv	Acquire sweep width optimized 2D inverse spectra.
au_getlxhco	Acquire sweep width optimized XH correlated spectra.
au_mult	AU program for C13 multiplicity analysis.
au_noediff	noe difference spectroscopy using different expnos.
au_noemult	noe difference spectroscopy with multiple irradiation points for each multiplet using different expnos.
au_water	Acquire water-suppression spectra for use in foreground (xau,xaua).
au_watersc	Acquire water-suppression spectra for use in automation, e.g., with sample changer.
au_zg	General AU program for data acquisition.
au_zg135	Acquire DEPT135 type spectra.
au_zgcosy	Acquire COSY type spectra.

au_zgglp	Automatic data evaluation according to GLP standards. This AU program takes O1, SW and O2 as arguments and then works like au_zg.
au_zgnr	Acquisition with rotation switched off.
au_zgonly	General AU program for data acquisition.
au_zgsino	Acquisition with signal to noise break up.
au_zgte	Acquisition with temperature setting.
aunmp_tojdx	Used in LIMS automation to process data. First, AUNMP is executed, then, if specified, the command given on the command line.
autoflist	Automatic generation of a frequency list for the peaks in the plot region of the spectrum.
autot1	Automatic processing of a 2D T1/T2 experiment with subsequent T1/T2 calculation.
bintoasc	Converts experiments from /<xwhome>/exp/stan/nmr/par containing old binary metafiles to an experiment which then contains the same plot parameters but in ASCII format.
bsms_exam	Example AU program which shows how to use low level functions to read or write BSMS parameters.
bsms_vtu_exam	Example AU program which shows how to use low level functions to read or write BSMS or VTU (BVT1000/BDTC) parameters.
butselau	Acquisition with butselnmr (buttonmr for selective experiments) from within XWIN-NMR.
buttonau	Acquisition with buttonnmr from within XWIN-NMR.
calcphhomo	Phase calculation program for noesytp, cosygsmftp, roesytp, mlevtp. Phase in F2 by reading and phasing ser file according to pulse program Phases in F1 are calculated.
calcphinv	Calculate the phase correction for the F1 dimension in HMQC/HSQC type experiments.
calcplen	Calculate the pulse length according to the power level.
calcpowlev	Calculate the power level according to the pulse length.

calctemp	Calculate the temperature in the probe using the chemical shift difference between the aliphatic and OH protons.
calfun	Calculates an FID from an arbitrary function. This AU program is especially useful when you want to create a user defined window function for the ’uwm’ command.
check-vtu	Updates TE variable from the actual temperature and store it in a separate file (edte) in the dataset.
cmdpanaux	Controls the start and function of command panels (see cpan command for more details).
coiltemp	Read the Shim Coil Temperature.
col_to_black	Set all colours to black that are defined for the current plot (NT only).
convto1d	Converts a 2D spectrum to 1D format.
decon_t1	Automatic deconvolution of a 2D T1/T2 experiment.
deptcyc	Creates 3 DEPT experiments from 13C experiment with CPD and then performs multiple cycles of NS scans (times 2 for DEPT90).
depthalt	Halt "deptcyc" AU program.
diffe	Calculate the difference spectra between expnos.
diffp	Calculate the difference spectra between procnos.
dosy	Setup for diffusion/DOSY experiments linear gradient amplitude ramp.
elim_ints	Eliminates regions from the intrng file that contain the solvent and/or reference signals. The result will be an intrng file where the integral trails have a more reasonable scaling and smaller integrals are better resolved.
f1ref	Corrects the referencing in F1 for inverse type experiments.
fidadd	Add up FID’s in incremented expno’s.
fidtoser	Writes a number of fids that are stored under the same NAME and incremental EXPNOs to a ser file.
getphsum	Reads the total phase values from the status parameters and stores them back to the actual parameters.

getti	
goalternate	Acquire alternated X/Y measurements. N averages are acquired alternatingly in two experiments.
graderror	
gontp	Starts an ntp test program.
gradpreemp	Preemphasis adjustment for gradient spectroscopy on AMX/ARX/ASX with gradient waveform memory.
gradprog	Set the relevant parameters and generate the necessary files for the execution of pulse programs containing up to ten shaped gradient pulses in three orthogonal directions. For AMX/ARX/ASX with gradient waveform memory.
gradratio	Calculates gradient ratios for common inverse gradient pulse programs.
gradratiogs	Calculates gradient ratios for common inverse gradient pulse programs.
gradshapes	Calculate various gradient shapes.
gradshimau	Start gradshim gradient shimming procedure.
gssel_setup	AU program to determine the transmitter offset for 1H selective gradient shimming using 1H as observe nucleus.
guide	Perform a remote request server for the 'NMR Guide and Encyclopedia' client.
gv	Returns the currently running xwinnmr version and the directory it is stored in.
humpcal	Performs the ’hump test’. Measures the width of a peak at 0.55% and 0.11% of its signal height.
hwcal	Calculate the width of a peak at half height.
iexpno	Program to change to a new experiment number.
ilhalt	Stop an interleaved acquisition which was started with the AU program interleave.
interleave	Perform interleaved acquisitions
jconv_aufx	Converts Jeol FX data in a loop. The data must be stored with increasing extensions like proton.1, proton.2, ... etc.

list_pp	Scans all experiment numbers of the current data set for the pulse program name and the first 30 characters of the title. All experiments that are found are listed on the screen. If an experiment is selected, then it is made the foreground data-set.
listall_au	Scans all AU programs and extracts the name and the short description. This information is then copied into the file listall in your home directory. This list corresponds to the list you are currently reading.
loadshimZ	Reads the on-axis shim values from disk and loads them to the BSMS.
lock_off	Switch off the lock to start data acquisition on the lock channel.
lock_on	Switch on the lock if it has been disabled.
loopadj	Parameter optimization au program which calculates the lock parameters loop filter, loop gain and loop time for optimal long-time stability after adjusting lock phase and lock gain to optimal.
make2d	Create a new 2D dataset from the current 1D dataset. Can be used for 2D spectroscopy andrelaxation experiments. F2 parameters are copied from the 1D data, F1 parameters are set to reasonable values.
mkflist	Automatically generates a frequency list file.
mulabel	Processing AU program for determination of 13C multiplicity.
multanal	Interactive AU program for determination of 13C multiplicity.
multext	Processing AU program for determination of 13C multiplicity
multi_decon	Automatic deconvolution of a series of 1D spectra with AI calibration.
multi_integ	Automatic integration of a series of 1D spectra with AI calibration.

multi_integ2	Automatic integration of a series of 1D spectra with calibration of the integral values.
multi_integ3	Automatic integration of a series of 1D spectra with AI calibration. The output is written in a format suitable for import in excel or similar desktop publishing programs.
multi_zgvd	Performs multiple acquisitions on increasing expnos with delays that are read from a vdlist file. Alternatively, a fixed delay can be entered.
multi_zgvt	Performs multiple acquisitions on increasing expnos with temperatures that are read from a vtlist file.
multicom	Executes an XWIN-NMR command in increasing expnos.
multicyc	Cycles through a series of acquisitions of increasing expnos.
multiefp	Performs multiple "efp" on increasing expnos.
multiexpt	Calculates experimental time for multizg.
multifp	Performs multiple "fp" on increasing expnos.
multiftapk	Performs multiple "ft;apk" on increasing expnos.
multihalt	Halt "multicyc" AU program.
multimas	Performs multiple MAS experiments on increasing expnos.
multipcom	Executes an XWIN-NMR command in increasing procnos.
multiwinpro	Performs multiple processing on increasing expnos. The program asks for the window function and its parameters.
multixfb	Performs multiple "xfb" on increasing expnos.
multizg	Performs multiple acquisitions on increasing expnos.
noediff	noe difference spectroscopy using different expnos.
noeflist	Automatic generation of a frequency list with the peaks from the current plot region for noe.
noemult	noe difference spectroscopy with multiple irradiation points for each multiplet using different expnos.
o1f1	Correct calibration of F1 axes in 2D MQ experiments of odd half integer nuclei.
paropt	Parameter optimization au program.

parray	Parameter optimization au program using parameter arrays. Derived from ’paropt’, but several parameters may now be changed per experiment. In addition, parameters are not changed via constant increments. Instead, the values are taken from an array.
pass2d	Perform a PASS experiment with 5 Pi-pulses and 16 increments (samples up to 16 spinning side bands).
pecosy	Program to pre-process P.E.COSY raw data before 2D-FT.
phtran	Transfer phase correction parameters PHC0 and PHC1 into acquisition parameters PH_ref and DE.
plintfac	Plot integrals with different scaling factors.
plot_3d	Plot planes of a 3D dataset.
plot_sino	Plot spectrum, scaling depends on Signal/Noise.
plot_to_file	Creates a postscript file of the desired plot.
poptau	Parameter optimization au program using parameter arrays. Derived from 'paropt' but several parameters can be optimized. The parameters are changed according to the parameter arrays.The AU program will be started from user interface 'popt' (parameter editor).
popthalt	Halt "popt" AU program.
pp2d	Performs a 2D peak picking with the help of the XWIN-NMR command "pp" for 1D spectra.
pp2dmi	Sets the peak picking parameter MI according to the parameter S_DEV and performs a 2D peak picking with the AU program "pp2d".
proc_1H	Processes and plots 1D spectra. Does not perform baseline correction.
proc_1d	Processes and plots 1D spectra. Uses 'autoplot' for plotting.
proc_1dapks	Processes and plot 1D spectra. Uses 'apks' for phase correction and 'autoplot' for plotting.
proc_1dconlf	Processes and plots 1D spectra. Uses 'autoplot' for plotting. Plots an additional spectrum on the same plot if there are peaks with a chemical shift > 11.

proc_1dconlf_pr	Processes and plots 1D spectra. Uses 'autoplot' for plotting. Plots an additional wq1spectrum on the same plot if there are peaks in the lowfield range outside the plot limits.
proc_1dexp	Processing AU program for 1D spectra with automatic expansions.
proc_1dglp	Processing AU program with automatic data evaluation according to GLP standards. This AU program takes CY as an argument and then works like proc_1d.
proc_1dinfo	Processes and plots 1D spectra. Uses 'autoplot' for plotting. Prints the info file ('edinfo') on the plot
proc_1dlf	Processes and plot 1D spectra. Uses 'autoplot' for plotting. Plots an additional lowfield plot.
proc_1dlfexp	Processing AU program for 1D spectra with additional low field plot and automatic expansions.
proc_1dpppti	Processes and plots 1D spectra. Creates a special peaklist file (frequency (Hz) and half width) and prints this on the plot. Uses 'autoplot' for plotting.
proc_1dppti	Processes and plots 1D spectra. Creates a peak picking list and prints this on the plot. Uses 'autoplot' for plotting.
proc_2d	Processing AU program for 2D spectra without plotting.
proc_2dhom	Processes and plots 2D homonuclear type spectra. Uses 'autoplot' for plotting.
proc_2dhom_2pp	Processes and plots 2D homonuclear type spectra with two positive projections. Uses 'autoplot' for plotting.
proc_2dinv	Processes and plots 2D inverse type spectra. Uses 'autoplot' for plotting.
proc_2dinv_2p	Processes and plots 2D inverse type spectra. Plots two projections. Uses 'autoplot' for plotting.
proc_2dpl	Processes and plots 2D type spectra. Uses 'autoplot' for plotting.
proc_2dsym	Processes and symmetrizes 2D type spectra. Uses 'autoplot' for plotting.

proc_2dt1	Automatic processing of a 2D T1/T2 experiment with subsequent T1/T2 calculation.
proc_cpd135	Processes and plots 13C CPD and DEPT135 spectra that were acquired with the AU program au_zg135. Uses 'autoplot' for plotting.
proc_glp	Automatic GLP data evaluation.
proc_intrng	Processes and plots 1D spectra. Uses the predefined integral range file 'testrng' for integration and 'autoplot' for plotting.
proc_no	AU program which does no processing.
proc_noe	Processes and plots noediff spectra. Uses 'autoplot' for plotting.
proc_t1	Automatic processing of a 2D T1/T2 experiment with subsequent T1/T2 calculation.
proc_tecalib	Evaluation of previous temperature calibration experiments.
psys180f1t1	Processing AU program for the 180 degree pulse calibration tests.
psysamp1s39	Processing AU program for the amplitude stability tests - with shaped pulse - with 30 degree pulse - with 90 degree pulse - after gradient echo (5msec, 30 G/cm) - after gradient echo (5msec, 10 G/cm) - after gradient pulse (1msec, 10G/cm).
psysb1hom	Processing AU program for the B1 homogeneity test.
psysb2hom	Processing AU program for the B2 homogeneity test.
psyscancel	Processing AU program for the - phase cycling cancellation test - phase cycling cancellation test after gradient pulse.
psysdante1	Processing AU program for the dante type turn on test.
psysdecpro1	Processing AU program for the decoupler profile test.
psysexpro1	Processing AU program for the - excitation profile (16 usec gauss shape) test - excitation profile (6 msec gauss shape) test.
psysglitch	Processing AU program for the glitch test.
psysgrreco1	Processing AU program for the gradient recovery test.

psysgrzpro	Processing AU program for the z-gradient profile.
psysmodl1	Processing AU program for the - modulator linearity test - shaped pulse modulator linearity test.
psysmultl1	Processing AU program for the amplitude linearity test (1dB power level steps).
psysphas1st	Processing AU program for the - phase stability test ("13 degree test") - shaped pulse phase stability test (16 usec gaussian shape, "13 degree test").
psysphasf1	Processing AU program for the - phase propagation test - phase shifting test.
psyspullin1	Processing AU program for the - amplitude linearity test - shaped pulse amplitude linearity test (pulse length *2, power level +6).
psysquadim	Processing AU program for the quad image suppression test.
psysrgtest	Processing AU program for the receiver gain test (analog and digital).
psyssoftp1	Processing AU program for the shaped pulse comparison (rectangular, gaussian, eburp1).
psystestab	Automatic processing of a 2D Temperature stability experiment, evaluation of temperature and statistic of temperature stability. Can be used to process data obtained with the AU program systestab.
psysturnon	Processing AU program for the turn on test.
pulse	Program to calculate attenuation value for given pulse length or nutation frequency, or vice versa.
pulsecalib	Offset/Pulsecalibration H2O/D2O and Offset/Pulsecalibration 13C, 15N probehead.
qnpset	Define the QNP parameter according to the currently defined probehead.
quadplot	First plots a 2D overview spectrum and then the 4 quadrants of the 2D spectrum.
queue	Queue data acquisition.
queue_init	Initialise data acquisition with the AU program queue.

queuerga	Queue data acquisition.
r23mplot	Read 2D slices from a 3D data set and plot them.
r23mult	Repeatedly reads slices from a 3D data set (3rrr) into successive experiment numbers.
rampXY	3D gradient shimming with the BSMS RCB board.
remproc	Automatic conversion and processing of data sets transferred via BRUKNET, LIGHTNET, NMR-LINK or TCP-LINK.
repeat	Repeat an acquisition with exactly the same parameters, pulse program and other lists.
secplot	Generate a section plot. The overview spectrum is plotted together with a vertical expansion of a smaller part of the spectrum on top of it.
selget	Import a shaped pulse into the current dataset.
selput	Export the current FID into a wave form file.
set2hdecgp	Setup AU program for standard 3D parameter sets.
setccnh3dgp	Setup AU program for standard 3D parameter sets.
setdiffparm	Extracts diffusion sequence parameters and stores parameters for "vargrad" simfit fitting (T1/T2) or DOSY processing.
seteditedgp	Setup AU program for standard 3D parameter sets.
sethccc3dgp	Setup AU program for standard 3D parameter sets.
setpar3dgp	Setup AU program for standard 3D parameter sets.
setproj	Sets the edg projection parameters to appropriate values.
set_sreglist	Set SREGLST parameter from NUC1 and SOLVENT.
shear	Program for 2D MQ experiments on nuclei with odd half integer spin for shearing the 2D spectrum after 2D FT.
showpp	Start NMR-SIM pulse program display. This program is used by the NMR guide&encyclopedia.
simplex	AU program for autoshimming. It is suitable for adjustment of strongly coupled shim groups which may be far from the optimum position.

simtoseq	Converts data which have been recorded in digital and qsim mode to data which appear to be acquired in qseq mode.
sinocal	Calculates the signal to noise ratio.
split2D	Splits a processed 2D file into single 1D spectra.
splitinvnoe	Separate NOE and NONOE data obtained with a pulse program like invinoef3gpsi.
splitser	Splits a ser file into single fids, starting with the expno which follows the ser file.
splitxf	Separate and combine double half filtered data.
stack1d	Generates a stacked plot of 1D spectra from increasing or decreasing EXPNOs or PROCNOs.
stack2d	Generate a 2D stack plot.
stackp1d	Generates a stacked plot of 3 to 12 1D spectra from increasing or decreasing EXPNOs or PROCNOs.
sti	Displays the title of the current dataset in a window without opening an editor (FAST!)
suppcal	Calculates the width of the Water peak at 100% and 50% of the DSS signal height. The result is referred to as the 'water suppression test'.
sys180f1t1	Acquisition AU program for the 180 degree pulse calibration test with different phases.
sys180f1t2	Acquisition AU program for the 180 degree pulse calibration test with different flip angles.
sysamp1sp9	Acquisition AU program for the shaped pulse amplitude stability test.
sysamp1st	Acquisition AU program for the amplitude stability tests - with 30 degree pulse - with 90 degree pulse.
sysb1hom	Acquisition AU program for the B1 homogeneity test.
sysb2hom	Acquisition AU program for the B2 homogeneity test.
syscancel	Acquisition AU program for the phase cycling cancellation test.
sysdante1	Acquisition AU program for the dante type turn on test.

sysdecpro1	Acquisition AU program for the decoupler profile test.
sysexpro1	Acquisition AU program for the - excitation profile (16 usec gauss shape) test - excitation profile (6 msec gauss shape) test.
sysgenpar	Preparation AU program for all HWT test programs.
sysglitch	Acquisition AU program for the glitch test.
sysgrcan	Acquisition AU program for the phase cycling cancellation test after gradient pulse.
sysgrecho	Acquisition AU program for the amplitude stability test after gradient echo (5msec, 30 G/cm and 5msec, 10 G/cm).
sysgrreco1	Acquisition AU program for the gradient recovery test.
sysgrstab	Acquisition AU program for the amplitude stability test after gradient pulse (1msec, 10G/cm).
sysgrzpro	Acquisition AU program for the z-gradient profile.
sysmodl1	Acquisition AU program for the modulator linearity test
sysmodls1	Acquisition AU program for the shaped pulse modulator linearity test.
sysmultl1	Acquisition AU program for the amplitude linearity test (1dB power level steps).
sysphas1sp	Acquisition AU program for the shaped pulse phase stability test (16 usec gaussian shape, "13 degree test").
sysphas1st	Acquisition AU program for the phase stability test ("13 degree test").
sysphasf1	Acquisition AU program for the - phase propagation test - phase shifting test.
syspullin1	Acquisition AU program for the amplitude linearity test (pulse length *2, power level +6).
sysquadim	Acquisition AU program for the quad image suppression test.
sysrgtest	Acquisition AU program for the receiver gain test (analog and digital).

syssoftp1	Acquisition AU program for the shaped pulse comparison (rectangular, gaussian, eburp1).
syssplin1	Acquisition AU program for the shaped pulse amplitude linearity test (pulse length *2, power level +6).
systestab	AU program for a temperature stability experiment performed as pseudo 2D experiment including evaluation of temperature and statistics of temperature stability.
systurnon	Acquisition AU program for the turn on test.
tecalib	AU program to determine the temperature calibration curve.
testsuite	Test the general functionality of an XWIN-NMR release version. Basic functionality is given if this program is completed without error messages.
tmscal	Performs a peak picking around the TMS signal. If the two satellites from the 29Si - 1H coupling can be detected, the resolution is OK.
tune	Tune a probehead.
update_layout	Sets the parameter 'LAYOUT' in all parameter sets.
update_aunmp	Sets the parameter AUNMP in all parameter sets.
vtu_exam	Example AU program which shows how to use low level functions to read or write VTU (BVT1000/BDTC) parameters.
writeshimZ	Reads the on-axis shim values and writes a pseudo shim file.
xfshear	Program for shearing of 2D MQMAS spectra of odd half integer quadrupolar nuclei. Data need to be acquired in States Mode
xwp_p1dlf	Processing AU program for 1D spectra with additional low field plot.AUTOPLOT (the automatic version of XWIN-PLOT) is used instead of XWIN-NMR's plot.
xwp_p2dpl	Processing AU program for 2D type spectra which don't need a symmetrization. AUTOPLOT (the automatic version *of XWIN-PLOT) is used instead of XWIN-NMR's plot.

xwp_pcpd135	Processing AU program for 13C CPD and DEPT135 spectra which were acquired with the AU program au_zg135. AUTOPLOT (the automatic version of XWIN-PLOT) is used instead of XWIN-NMR's plot.
zeroim	Zeroe the imaginary data of a 1D or 2D data set.
zg_2Hoffon	General AU program for data acquisition. The lock is switched off before the acquisition is started.
zgchkte	Starts acquisition with zg and monitors the temperature. The experiment is halted if the current temperature differs too much from the target temperature.
zg_dfs	Calculates shape file for double frequency sweep and subsequent data-acquisition.
2df1shift	Shift a 2D spectrum along the F1 axis.
2dgetref	Gets parameters for a 2D spectrum from the 1D reference spectra : Nucleus, Frequencies, Spectral Width, and reference plot data set names. The F2 reference is taken from the second dataset. The F1 reference is taken from the third dataset.
2dshift	Shift 2D time domain data left or right over NSP points.
2nde	Set 2nd data set to new expno and 3rd data set equal to foreground data set.
2ndn	Set 2nd data set to new name and 3rd data set equal to foreground data set.

Chapter 13

XWIN-NMR parameter types

This chapter contains a list of all XWIN-NMR parameters grouped by their type. The type of a parameter can be integer, float, double or character-string. Several AU macros read XWIN-NMR parameters into AU variables or store the value of AU variables into XWIN-NMR parameters. In both cases it is important that the type of the AU variable is the same as the parameter type.

13.1 Integer parameters

ABSG	AQORDER	AQSEQ	AQ_mod
BC_mod	BYTORDA	BYTORDP	DATMOD
DIGMOD	DIGTYP	DS	EXPNO2
EXPNO3	FL1	FL2	FL3
FL4	FnMODE	FS[8]	FT_mod
HL1	HL2	HL3	HL4
HGAIN[4]	HOLDER	HPMOD[8]	HPPRGN
INTBC	L[32]	LOCSHFT	LPBIN
MC2	ME_mod	NBL	NC
NCOEF	NC_proc	NLEV	NS
NSP	NTH_PI	NZP	OVERFLW
PAPS	PARMODE	PHP	PH_mod
PKNL	POWMOD	PPARMOD	PR
PRGAIN	PSCAL	PSIGN	PROCNO2
PROCNO3	QNP	REVERSE	RO
RSEL[10]	S[8]	SEOUT	SI
STSI	STSR	SURQMSG	SYMM
TD	TD0	TDeff	TDoff
TILT	TUNHIN	TUNHOUT	TUNXOUT
WBST	WDW	XDIM	XGAIN[4]
XL	YL	YMAX_a	YMAX_p
YMIN_a	YMIN_p		

The following XWIN-NMR parameters are of the type integer:

13.2 Float parameters

The following XWIN-NMR parameters are of the type float:

ABSF1	ABSF2	ABSL	ALPHA
ASSFAC	ASSFACI	ASSFACX	ASSWID
AZFE	AZFW	BCFW	CNST[32]
DBL[8]	DBPOAL[8]	DBPOFFS[8]	DBP[8]
DC	DE	DL[8]	DPOAL[8]
DPOFFS[8]	DP[8]	D[32]	FCOR
FOV	FW	GAMMA	GB
GPX[32]	GPY[32]	GPZ[32]	INTSCL
ISEN	LB	LEV0	LOCPHAS
MASR	MAXI	MI	NOISF1
NOISF2	OFFSET	PC	PCPD[10]
PHC0	PHC1	PHCOR[32]	PH_ref
PL[32]	P[32]	RECPH	RG
SIGF1	SIGF2	SINO	SPOAL[32]
SPOFFS[32]	SP[32]	SSB	S_DEV
TE	TE2	TL[8]	TM1
TM2	TOPLEV	TPOAL[8]	TPOFFS[8]
TP[8]	V9	VD	ZL1
ZL2	ZL3	ZL4	

13.3 Double parameters

The following XWIN-NMR parameters are of the type double:

BF1	BF2	BF3	BF4
BF5	BF6	BF7	BF8
COROFFS	CY	F1P	F2P
INP[32]	IN[32]	LFILTER	LGAIN
LOCKPOW	LTIME	O1	O2
O3	O4	O5	O6
O7	O8	SF	SFO1
SFO2	SFO3	SFO4	SFO5
SFO6	SFO7	SFO8	SW
WBSW			

13.4 Character-string parameters

The following XWIN-NMR are of the type character-string:

AUNM[16]	AUNMP[16]	CPDPRG[16]	CPDPRGB[16]
CPDPRGT[16]	CUREXP[32]	CURPLOT[80]	CURPRIN[80]
DBPNAM0[16]	DECBNUC[8]	DECNUC[8]	DFILT[16]
DFORMAT[16]	DPNAME0[16]	DSLIST[16]	DU[256]
DU2[256]	DU3[256]	EXP[32]	F1LIST[16]
F2LIST[16]	F3LIST[16]	FQ1LIST[16]	GPNAM0[64]
GRDPROG[16]	INSTRUM[16]	LAYOUT[256]	LFORMAT[16]
LOCNUC[8]	MASRLST[16]	NAME[64]	NUC1[8]
NUCLEUS[8]	PFORMAT[16]	PROBHD[64]	PULPROG[16]
SOLVENT[32]	SPNAM0[64]	SREGLST[40]	TI[72]
TPNAME0[16]	TYPE[16]	USER[64]	USERA1[80]
USERP1[80]	VCLIST[16]	VDLIST[16]	VPLIST[16]
VTLIST[16]			

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