BRUKER

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Pulse Programming

Manual for TopSpin 2.1

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Pulse Programming

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Chapter 1

Basic pulse program writing

1.1 Introduction

A pulse program is an ASCII text consisting of a number of lines. Each line may contain one or more pulse program statements which specify actions to be performed by the acquisition hardware and software. You can set up a pulse program with the XWIN-NMR commands *edpul* or *edcpul* (see the Acquisition Reference manual). The XWIN-NMR acquisition commands *gs*, *go*, and *zg* execute the pulse program defined by the acquisition parameter PULPROG which can be set with *eda* or *pulprog*. Pulse program execution is a two-step process: After entering *gs*, *go*, or *zg*, the *pulse program compiler* is invoked which translates the pulse program text into an internal binary form that can be be executed. Possible syntax errors are reported. If errors are found, the acquisition will not be started. If, however, the compilation is successful, the compiled pulse program is loaded into the acquisition hardware and the measurement begins.

Spectrometer naming conventions

This manual is written for AV spectrometers. Nevertheless, a large part of it is also valid for older spectrometers like AMX, ARX, ASX, and Avance. You can easily find out which type of spectrometer you have at the cabinet

door; the name is AV, AV II or AV III (sometimes also AV II+)

1.2 Pulse program library

Routine users normally use Bruker pulse programs that delivered with TOP-SPIN. The **edpul** command displays a list of these pulse programs and allows you to view their contents. Viewing Bruker pulse programs requires that the **expinstall** command was executed once after the installation of TOPSPIN. This command copies the pulse programs suitable for your spectrometer into the data bank.

If you want to write your own pulse programs, it can be helpful to start with a Bruker pulse program and modify it to your needs.

1.3 Pulse program display

A graphical representation of a pulse program for AV spectrometers can be obtained with the command **spdisp**, which is described in the Acquisition Reference manual.

The command **hpdisp,** which is also described in the Acquisition Reference manual, displays the pulse program showing the signals as produced by the spectrometer hardware with exact timing of pulses, phases and amplitudes.

1.4 Basic syntax rules

Table 1.1 shows *zgcw30* as an example of a simple Bruker pulse program. Here the following pulse programming rues are used:

1. Pulse programs are *line oriented*. Each line specifies an *action* to be performed by the acquisition hardware or software.

2. A semicolon (;) indicates the beginning of a comment. You can put it anywhere in a line. The rest of the line will then be treated as a comment.

3. #include <filename> or #include "filename"
This statement allows you to use pulse program text that is stored in a

```
;zgcw30
;avance-version
;1D sequence with CW decoupling
;using 30 degree flip angle

#include <Avance.incl>

1 ze
  d11 pl26:f2
  d11 cw:f2
2 d1
  p1*0.33 ph1
  go=2 ph31
  wr #0
  d11 do:f2
  exit

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

;pl1 : f1 channel - power level for pulse (default)
;pl26: f2 channel - power level for cw/hd decoupling
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
;d11: delay for disk I/O [30 msec]
```

Table 1.1 Pulse program example

different file. It allows you to keep your pulse program reasonably sized, and to use the same code in various pulse programs. If the filename is given in angle brackets (< >), the file is searched for in the directory *$XWINNMRHOME/exp/stan/nmr/lists/pp/*. Alternatively, double quotes (" ") can be used to specify the entire path name of the file to be included.

4. 1 ze
Any pulse program line can start with a *label* ("1" in the example above). Labels are only required for lines which must be reached by loop or branch statements such as go=label, lo to label times n or goto label. You can, however, also use labels for numbering the lines. A label can be a

number or, an alphanumeric string followed by a comma. An example of the latter is:

> firstlabel, ze

The statement ze has the following function:

- Reset the *scan counter* (which is displayed during acquisition) to 0
- Enable the execution of *dummy scans.* This will cause the pulse program statement go=label to perform DS dummy scans before accumulating NS data acquisition scans. If you replace ze with zd, go=label will omit the dummy scans
- The statement zd automatically resets all program pointers to the first element, whereas the statement ze sets all phase program pointers such that they are at the first element after DS dummy scans.

5. d11 pl14**:**f2
Execute a delay whose duration is given by the acquisition parameter D[11]. Behind any delay statement, you can specify further statements to be executed during that delay (note that the delay must be long enough for that statement). In this example, the power level of channel f2 is switched to the value given by the acquisition parameter PL[14].

6. d11 cw:f2
Execute a delay whose duration is given by the acquisition parameter D[11] and, at the same time, turn on continuous wave (cw) decoupling on frequency channel f2. Decoupling will remain active until it is explicitly switched off with the statement do**:**f2. This delay and cw decoupling will begin immediately with the delay on which it is specified.
Items 5 and 6 illustrate a general feature of pulse programs: the actions specified in two consecutive lines are executed sequentially. Actions specified on the same line are executed simultaneously.

7. 2 d1
Execute a delay the duration of which is given by the acquisition parameter D[1]. This line starts with the label "2", the position where the statement go=2 will loop back to.

8. p1*0.33 ph1
Execute a pulse on frequency channel f1. The pulse length of this pulse is given by the acquisition parameter P[1] multiplied by 0.33. P[1] is nor-

mally used for the pulse width of a 90° flip angle. The statement p1*0.33 would then execute a 30° pulse. In general, you can specify the operator * behind (not before!) a pulse or delay statement, followed by a floating point number. Note that the channel f1 is not specified; it is the default channel for p1, i.e.:

    p1*0.33

is identical to:

    p1*0.33**:f1**

The pulse is executed with a power (amplitude) defined by the acquisition parameter PL[1]. PL[1] is the default power level for channel f1, but you can also use a different parameter. For example, the statement pl7**:f1** sets the channel f1 power to the value of PL[7]. It must be put on a separate line, with a delay, before the line with the pulse statement.

The phase of this pulse in our example is selected according to ph1, the name of a *phase program* or *phase list*. It must be specified behind the pulse and defined after the pulse program body. In this example we use the phase program

    ph1=0 2 2 0 1 3 3 1

The phase of the pulse varies according to the current data acquisition scan. For the first scan, p1 will get the phase *0*90°*, for the second scan *2*90*, for the third scan *2*90*, for the fourth scan *0*90,* etc. After 8 scans, the list is exhausted. The phase program is cycled so with scan 9 the phase will be set to the first element of the list: *0*90°*. Phase cycling is a method of artefact suppression in the spectrum to be acquired. The receiver phase must be cycled accordingly to ensure that coherent signals of subsequent scans are accumulated, not cancelled. This is achieved by the receiver phase program ph31 in our example.

9. go=2 ph31
Execute one data acquisition scan, then loop to the pulse program line with label "2". Repeat this until NS scans have been accumulated. Note that NS is an acquisition parameter. The data acquisition scans are preceded by DS *dummy scans* (because the statement ze is used at the beginning of the pulse sequence rather than zd). A *dummy scan* does not acquire any data, but requires the same time (given by the acquisition parameter AQ) as a real scan. Dummy scans are used to put the

spin system of the sample into a steady state before acquisition starts. The receiver phase is changed after each scan as described above for the pulse phase. Phase cycling is done according to the phase program ph31. Phase cycling is also used during the execution of dummy scans. Both DS and NS must therefore be a multiple of the number of phases in the list.

The go=label statement executes a delay, the so-called *pre-scan delay* to avoid pulse feed through before it starts digitizing the NMR signal. During this time the receiver gate is opened. For AQ_mod = DQD and for any value of AQ_mod if you have an RX22 receiver, the frequency is switched from *transmit* to *receive*. DE is an acquisition parameter that can be set from *eda* or by entering *de* on the command line. It consists of the sub-delays DE1, DE2, DEPA, DERX and DEADC that can be set with the command *edscon* (see the Acquisition Reference manual). Normally, you can accept the default values for DE value and its sub-delays. The total time the go=label statement requires to execute a scan is DE+AQ+3 millisec. The duration of 3 millisec is required for preparation of the next scan. It is valid for all Avance type spectrometers.

wr #0
Writes the accumulated data as file *fid* into the EXPNO directory of the current data set. Note that with the *zgcw30* pulse program, data are only stored on disk after all NS scans have been accumulated. You can, however, store the data to disk after any scan during the acquisition by entering the command *tr* on the command line. You can process and plot these data while the acquisition continues. If you want to protect your data against power failures during long term experiments, we recommend that you write the data on disk in regular intervals, for example every 100 scans. To accomplish this, you can set NS=100 and TD0=300 (if the pulse program is written using the mc-syntax). The pulse program then accumulates a total of 30.000 scans, but stores the result every 100 scans.

Please note that the loop must include the ze statement. The reason for this is that wr #0 *adds* the last acquired data to the data already present in the file.

The real time FID display will only show the data currently present in the acquisition processor's memory.

10.exit

Specifies the end of the pulse program.

1.5 **Pulse generation**

Table 1.2 shows the available types of statements for the generation of high frequency pulses.

p0, p1, ... , p63	Generate a pulse whose length is given by the acquisition parameter P[0], ..., P[63].
p0:r, ...,p63:r	Generate a pulse whose length is given by the acquisition parameter P[0], ..., P[63] and which is randomly varied. The maximum variation (in percent) is defined by the acquisition parameter V9.
3.5up, 10mp, 0.1sp	Generate a pulse of fixed length: up = a μsec pulse (mp = millisec, sp = sec).
P135, p30d1H	Generate a pulse, whose name is defined by a define pulse statement, and whose duration is defined by an expression.
vp	Generate a pulse whose length is taken from a pulse list.

Table 1.2 Pulse generation statements

A high frequency pulse is described by its:

- duration (= pulse width)
- frequency
- phase
- power (= amplitude) and shape

The following paragraphs will describe these items.

1.5.1 Pulse duration

The pulse duration is selected according to the name of the pulse statement.

1.5.1.1 p0-p63

The statement:

    p0

executes a pulse of width P[0]. P[0] is an acquisition parameter that can be set from *eda*, or by typing *p0* on the command line. Likewise, the statement:

    p1

executes a pulse of width P[1].

1.5.1.2 Fixed length pulses

The statement:

    10mp

executes a pulse of width 10 millisec (called a *fixed pulse* because its duration cannot be manipulated, see below). The duration must be followed by up, mp or sp. These units indicate microseconds, milliseconds, and seconds, respectively. If you would omit the terminating "p", a delay would executed instead of a pulse.

1.5.1.3 Random pulses

The statement:

    p0:r

executes a pulse of length P[0] which is varied randomly. The parameter V9 specifies, in percent, the maximum amount which is added to or subtracted from P[0]. As such, the effective pulse varies between 0 and 2*P0. It can be set from *eda*, or by typing *v9* on the command line.

Please note that the *gs* command ignores the :r option.

1.5.1.4 User defined pulses

The statement:

p30d1H

executes a pulse whose name is defined by the user, and whose duration is determined by an arithmetic expression. For example, the line:

define pulse p30d1H

defines p30d1H to be a pulse statement, and the line:

"p30d1H=p1*0.33"

defines the expression for its duration. Note that the definition must be within double-quotes (") .

Both the *define* statement and the defining expression must be placed before the beginning of the actual pulse sequence. It is evaluated at compile time of the pulse program, not at run time. User defined pulses can consist of alphanumeric characters, where the first character must be a alphabetic. The maximum length of the name is 11 characters. Make sure you do not use any of the reserved words like ‚adc', ‚go', ‚pulse' etc.

1.5.1.5 Variable list pulses (obsolete)

The statement:

vp

executes a pulse whose duration is given by the current value of a *pulse list*. A pulse list is a text file that contains one pulse duration per line. It can be set up with the command **edlist** (described in the Acquisition Reference manual). The statement vp uses the list file given by the acquisition parameter VPLIST. When the pulse program begins, the first duration in the list is used. The statement ivp moves the list pointer to the next duration. If the end of the list is reached, the pointer is set to the first item. The statement ivp must be specified behind a delay, for example:

d1 ivp
0.1u ivp

The length of the delay is irrelevant; any value is allowed.

You can also set a specific list position with an equation. For example:

    "vpidx=5"
    vp

The statement vp will execute the pulse defined at position 5 of the pulse list. To the right of the equal sign, any dimensionless expression is allowed. It may contain any of the parameters listed in Table 1.3.

1.5.1.6 Pulse lists defined in the pulse program

Instead of setting up a pulse list with **edlist**, a list of pulses can also be specified within the pulse program using a define statement, e.g.:

    define list<pulse> Plist = { 10 20 30 }

This statement defines the pulse list Plist with values 10 msec, 20 msec and 30 msec. User defined pulse lists must be initialized within the definition. There are two alternatives to assigning values directly in {}-brackets. You can specify the filename of a pulse list or the variable that contains such a filename, both in angle brackets. Examples,

    define list<pulse> P2list = <mypulselist>

    define list<pulse> P3list = <$VPLIST>

In both cases, the file that contains the pulse list can be created with the command **edlist vp**.

According to the define statements above:

    P1list

executes a pulse of 10 msec the first time it is invoked. In order to access different list entries, you can append the **.**inc, **.**dec or **.**res postfix to the pulse statement to increment, decrement or reset the index, respectively. Any index operations are performed cyclically i.e. when the pointer is at last entry of a list, the next increment will move it to the first entry. Furthermore, list entries can be specified directly in squared brackets counting from 0, i.e. the statement:

    P1list[1]

executes a pulse of 20 msec according to the above definition. Lists can be executed and incremented with one statement, using the caret postfix

operator. As such, the statement:

    P1list^

is equivalent to:

    P1list P1list.inc

Finally, you can set the index directly in an arithmetic expression within double quote characters, appending .idx to the pulse statement. The following example shows the use of a pulse list that is assigned within its definition:

    define list<pulse> locallist = {10 20 30 40}

    locallist locallist.inc   ; pulse of 10 msec, change index from 0 to 1
    locallist locallist.res   ; pulse of 20 msec, set index to 0
    locallist[2]   ; pulse of 30 msec (do not interpret the index)
    locallist locallist.dec   ; pulse of 10 msec, change index from 0 to 3
    locallist   ; pulse of 40 msec
    "locallist.idx = 3"   ; set index to 3
    locallist^   ; pulse of 40 msec, move index to 0
    locallist   ; pulse of 10 msec

<u>Caution</u>: index operations on pulse lists only take effect in the next line. Furthermore, you cannot access two different entries of the same list on one line. This is illustrated in the following example:

    define list<pulse> locallist = {10 20 30 40}

    locallist^ locallist   ;uses the same list entry (10 ms) twice
    locallist   ;the ^ operator takes effect: 20ms
    locallist[2] locallist[3]   ;executes locallist[3] (40 ms) twice

Note that names for user defined items may consist of up to 19 characters, but only the first 7 are interpreted: i.e Pulselist1 and Pulselist2 are allowed names but they would address the same symbol.

1.5.1.7 Manipulating pulse durations: The operator "*"

A pulse duration can be manipulated with the operator "*". Examples of allowed statements:

> p1*1.5
>
> p30d1H*3.33
>
> p3*oneThird
>
> vp*3

The operator must be placed behind the pulse statement. *oneThird* is the name of a macro which must have been defined at the beginning of the pulse program, e.g.:

> #define oneThird 0.33

Note that fixed pulses cannot be manipulated. So the statement 10mp*0.33 would be incorrect.

1.5.1.8 Manipulating pulse durations: Changing p0-p31 by a constant value

Each pulse statement p0-p31 has been assigned an acquisition parameter INP[0]-INP[31] These parameters take a duration value, in msec. The pulse program statements ipu0-ipu31 add the value of INP[0]-INP[31] to the current value of p0-p31, respectively. Likewise, dpu0-dpu31 subtract the value of INP[0]-INP[31] from the current value of p0-p31. The statements rpu0-rpu31 reset p0-p31 to their original values, i.e. to the values of the parameters P[0]-P[31]. The statements presented in this paragraph must be specified behind a delay of any length (³ 0) . Some examples:

> d1 ipu3
> 0.1u dpu0
> d1 rpu0

1.5.1.9 Manipulating pulse durations: Redefining p0-p63 via an expression

The duration of the pulses p0-p63 is normally given by the parameters P[0]-P[63]. You can, however, replace these values by specifying an expression in the pulse program. The following examples show how you can do this:

> "p13=3s + aq - dw*10"
> "p13=p13 + (p1*3.5 + d2/5.7)*td"

The result of such an expression must have a time dimension. You can therefore include acquisition parameters such as pulses, fixed pulses, delays, fixed delays, the acquisition time AQ and the dwell time DW within the expression. Furthermore, you can include parameters without a dimension such as the time domain size TD. The complete list is shown in Table

d0-d31 [sec]
p0-p31 [μsec]
l0-l31 (loop counters)
in0-in31[sec]
inp0-inp31 [μsec]
aq [sec]
dw [μsec]
dwov [μsec]
de1, depa, derx, deadc [μsec]
vd [sec]
vp [μsec]
nbl, ds, ns, nsdone, td, td1, td2
decim
cpdtim1-cpdtim8 [sec]
cnst0-cnst31

Table 1.3

1.3.

An expression must be specified between double quote characters (" "). It can be placed anywhere in the pulse program, as long as it occurs before the line that contains the corresponding pulse statement (which would be p13 in our example). Note that the second expression in the example above assigns a new value to p13 each time the expression is encountered, e.g. if it is contained in a pulse program loop.

Expressions cannot be used in labelled pulse program lines. You can, how-

ever, put a small duration behind a label and put the expression in the next line.

Expressions do not cause an extra delay in the pulse program. Pre-evaluation is applied before the pulse program is started, and the result is stored in the available buffer memory to be accessed at run time. At run time, pre-evaluation is performed during the cycle time of the loops in which the statements are embedded. If loops are executed too fast, a run time message is printed.

1.5.1.10 Manipulating the durations of user defined pulses

User defined pulses, as described in section 1.5.1.4, can be manipulated in the same way pulses defined by p0-p63 are manipulated (see sections above).

1.5.2 Pulse frequency

1.5.2.1 Frequency channels

The RF frequency of a pulse is selected via the spectrometer channel numbers f1, ... ,f8 (the actual numbers of the channels depend on your spectrometer type and accessory). A pulse on a particular channel is executed with the frequency defined for that channel. The statements:

> p1**:f2**
>
> p2*0.33**:f2**
>
> p30d1H*3.33**:f2**
>
> vp**:f2**

all execute a pulse on channel f2, with the duration P[1], P[2]*0.33, p30d1H*3.33 and a values from VPLIST, respectively. The pulse frequency is the value of the acquisition parameter SFO2; the default frequency for channel f2. If the channel is not specified in the pulse statement, p1, p2, ..., p31 all use the default channel f1. The default frequencies of the channels f1-f8 are given by the parameters SFO1-SFO8 (see the description of SFO1, NUCLEI, and *edasp* in the Acquisition Reference manual for more information about defining frequencies for a particular channel). These parameters are loaded into the synthesizer(s) before the pulse program

starts. This gives the hardware time to stabilize before the experiment begins.

1.5.2.2 Using frequency lists

You can change the frequency of a channel within a pulse program with the statements fq1-fq8. They take the current value from a frequency list. A frequency list is a text file whose lines contain frequency values (see the command ***edlist*** in the Acquisition Reference manual). For example, the statement:

    d1 fq2**:**f3

which is equivalent to:

    d1 fq=fq2**:**f3

uses the frequency list whose file name is defined by the acquisition parameter FQ2LIST (fq1 would use FQ1LIST, etc.). You can set FQ1LIST etc. from the ***eda*** dialog box, and you can modify a selected list with ***edlist***. The example above sets the frequency of channel f3 by taking the *current* value from the list defined by FQ2LIST. When fq2 is executed the first time, the *current* value is the first value in the list . The next time fq2 is encountered (e.g. because it occurs several times in the pulse program, or because it is contained in a loop) the current value will be the next value in the list, etc. At the end of the list, the pointer will be set to the first entry of the list. The statements fq1-fq8 not only set a frequency, but also increment the list pointer to the next entry of the list. The list can, optionally, contain a frequency offset in MHz. If it does, the frequency list values in Hz are added to this offset. If it doesn't, the list values are added to the channel frequency (SFO1 for f1, SFO2 for f2, etc.).

The frequency can also be set to the values of the parameters CNST0-31 or to any number, for example:

    d1 fq=cnst20:f1   ; SFO1 [MHz] + CNST[20] [Hz]

    d1 fq=3000:f1   ; SFO1 [MHz] + 3000[Hz]

set the frequency on channel f1 to the value of CNST20 and to 3000 Hz, respectively. The default settings refer to SFOn as base frequency and the offsets are in Hz. But the offset can be given in PPM as well, and the base

channel frequency can be BFn instead of SFOn. This is achieved by specifying options after the frequency setting command. Example:

        d1 fq=cnst20 (bf ppm):f1

The resulting frequency will be Fn = BFn[MHz](1 + 1.0e-6*CNST[20][PPM]). The following options are possible:

Option	Meaning
sfo	base frequency SFOn
bf	base frequency BFn
hz	offset in Hz
ppm	offset in ppm

Table 1.4 frequency command options

1.5.2.3 Frequency lists applied to the reference frequency

The reference frequency is the intermediate frequency which is used by the receiver to mix the observed signal down to a lower frequency which can be digitized there. Normally this frequency is the same as the frequency of the transmitter pulse (except for DQD). If this frequency must be changed during pulse program execution, use the (receive) option, like for instance:

        1u FQ1(receive):f1

1.5.2.4 Frequency lists defined in the pulse program

For AV spectrometers, frequency lists can also be defined in the pulse program using the define statement. The name of a list can be freely chosen, for example:

        define list<frequency> username = { 200 300 400 }

The list must be initialized, specifying a list of frequency offsets between braces, separated by white spaces. By default, the entries are taken as frequency offsets (in Hz) to the default frequency (SFOx) of the channel, for which the list is used. However, this behaviour can be changed by specifying a modifier before the first entry of the list, e.g.:

        define list<frequency> absfq = {O,300.13,4000,5000,6000}

The modifiers are shown in the following table.

O <basic frequency [MHz]>	offset is in Hz and relative to basic freq. O
p (lower case)	offset is in PPM and relative to SFOx
P (upper case)	offset is in PPM and relative to BFx
no modifier	offset is in Hz and relative to SFOx

Table 1.5 deprecated modifiers in frequency lists

The usage of these modifiers is deprecated now. Instead the options from table 1.4 should be specified before the first element, separated by a comma:

define list<frequency> absfq = {ppm bf, 4000, 5000, 6000}

Instead of list entries, a list definition can also contain the name of a list file between angle brackets, e.g.:

define list<frequency> filefq = <freqlist>

The specified file can be created with the command *edlist f1*. Alternatively, you can specify $FQxLIST between angle brackets, where x is a digit between 1 and 8. For example:

define list<frequency> f1list = <$FQ1LIST>

In this case the value of the parameter FQxLIST will be used as filename. The format of frequency lists is the following: the first line contains the modifiers according to either table 1.4 or 1.5, the following lines contains the frequencies, one item per line.

A maximum of 32 different frequency lists can be defined within a pulse program. The name can be of arbitrary length, but only the first 7 characters are interpreted.

A difference between a regular frequency lists (interpreted by the fq*n* statements) and a frequency list defined within the pulse program is that the latter is *not autoincremented*. The list index can, however, be manipulated with postfix operators. The operators **.**inc, **.**dec, **.**res increment, decrement and reset the index, respectively. Furthermore, you can use a caret operator (**^**) to execute the list and increment the pointer with one statement. You

can also address a list entry by specifying its index in square brackets [].
Note that index manipulation statements are executed at the end of the
duration. This, for example, means that the statement:

    d1 fqlist^**:**f1 fqlist**:**f2

sets both channels f1 and f2 to the same frequency and afterwards incre-
ments the list pointer.

Note that the index runs from 0 and will be treated modulo the length of the
list. As such, by incrementing the index, the frequency can be cycled
through a list.

You can also set the index with a relation adding the **.**idx postfix to the list
name.

Example:

```
define list<frequency> fqlist = { 100 200 300}
ze
1 p1
  d1 fqlist:f1 fqlist.inc          ; set freq. to SFO1+100, incr. pointer
  p1:f1                           ; use frequency SFO1+100Hz
  d1 fqlist^:f1                   ; set frequency and increment
pointer
  p1:f1 fqlist.res                ; use freq. SFO1+200, set pointer to
0
  d1 fqlist:f1                    ; set frequency to SFO1+100
  p1:f1                           ; use frequency SFO1+100
    d1 fqlist[2]:f1               ; set frequency to SFO1 +300
  p1:f1                           ; use frequency SFO1+300
    "fqlist.idx = 1"             ; set pointer to entry 1
  d1 fqlist:f1                    ; set the frequency SFO1+200
  p1:f1                           ; use frequency SFO1+200
  d1 fqlist.dec                   ; decrement pointer
  go=1
exit
```

1.5.3 Pulse phase

1.5.3.1 Phase programs: definition

Pulse phases are relative phases with respect to the reference phase for signal detection. A phase must be specified behind a pulse statement with the name of a *phase program*. For example, the statements:

```
10mp:f1 ph3
p2*0.33:f2 ph4
p30d1H*3.33:f3 ph5
vp:f4 ph6
```

execute pulses on the channels f1, f2, f3 and f4, respectively. As such, the channel frequencies would be SFO1, SFO2, SFO3, and SFO4. The channel phases are set according to the current value of the *phase programs* ph3, ph4, ph5, and ph6, respectively. If a pulse is specified without a phase program, it will have the last phase that was assigned to the channel on which the pulse is executed. Note that at pulse program start, before any pulse has been executed, the phase on all channels is zero.

The four examples above can also be written in the following form:

```
(10mp ph3):f1
(p2*0.33 ph4):f2
(p30d1H*3.33 ph5):f3
(vp ph6):f4
```

This form expresses more clearly that a phase is a property of a spectrometer channel.

1.5.3.2 Phase programs: syntax

A phase program can be specified as shown in the following examples:

```
ph1 = 0 0 1 1 2 2 3 3                        ;(1)
ph1 = (5) 0 3 2 4 1                          ;(2)
ph1 = {0}*4 {2}*4                            ;(3)
ph1 = {0 2}^1                                ;(4)
ph1 = {0 2}^1^2^3                            ;(5)
ph1 = {1 3}^1^2*2                            ;(6)
ph1 = {{0 2}*2}^1^2                          ;(7)
ph1 = {{{0}*2}^2^3^1}^2                      ;(8)
```

```
ph1 = (5) {1 2}*2^1                                 ;(9)
ph1 = ph2*2 + ph3                                   ;(10)
ph1 = (float, 90.0) 30 60 95.5                      ;(11)
```

A phase program can contain an arbitrary number of phases.

Furthermore, the list of phases in a phase program can be spread over several lines, for example:

```
ph1 = 0 2 2 0
      1 3 3 1
```

In (1), the phases are expressed in units of 90°. The actual phase values are 0, 0, 90, 90, 180, 180, 270, 270.

In (2), the phases are expressed in units of 360/5 degrees, corresponding to the actual phase values 0*72, 3*72, 2*72, 4*72, 1*72 = 0, 216, 144, 288, 72 degrees. The divisor, to be specified in parentheses ( ) and before the actual phase list, can be as large as 65536 (corresponding to 16 bits). This corresponds to a digital phase resolution of 360/65536, which is better than 0.006°.

In (3) - (9), the operators " * " and " ^ " are used, which allow you to write long phase programs in a compact form. For phase programs with less than 16 phases, the explicit forms (1) and (2) are usually easier to read. The operator "*n" (with n = 2, 3, ...) must be specified behind a list of phases that is enclosed in braces { }. It repeats the contents of the braces (n-1) times. The operator "^m" (with n = 1, 2, 3, ...) must be specified behind a list of phases that is enclosed in braces { }, or behind a previous "^m" or behind an "*" operator. Each "^m" operator repeats the contents of the braces exactly once, but the repeated phase list will be incremented by m*360/d degrees (modulo d) where d is the divisor of the phase program. If no divisor is specified, the default value of 4 is used. The following lines display the phase programs (3) - (9) in their explicit forms:

```
ph1 = 0 0 0 0 2 2 2 2                               ;(3')
ph1 = 0 2 1 3                                       ;(4')
ph1 = 0 2 1 3 2 0 3 1                               ;(5')
ph1 = 1 3 2 0 3 1 1 3                               ;(6')
ph1 = 0 2 0 2 1 3 1 3 2 0 2 0                       ;(7')
ph1 = 0 0 2 2 3 3 1 1 2 2 0 0 1 1 3 3               ;(8')
ph1 = (5) 1 2 1 2 2 3                               ;(9')
```

In (10), the phase program is the sum of two other phase programs, one of which is multiplied with an integer constant. This principle is illustrated by the following example. Assume the following phase programs:

    ph2 = 0 2 1 3
    ph3 = 1 1 1 1 3 3 3 3

In order to calculate ph5 = ph2*2 + ph3, we first calculate ph2*2:

    ph2*2 = 0 0 2 2

Then we extend ph2 to the same size as ph3:

    ph2 = 0 0 2 2 0 0 2 2
    ph3 = 1 1 1 1 3 3 3 3

Now we calculate the sum of the two:

    ph1 = 1 1 3 3 3 3 1 1

In cases where phase programs are added and the size of one of them is not a multiple of the size of the other, the resulting phase program will have the length of the smallest common multiple of the two phase programs.

In (11), the phases are defined as floating point numbers in degree. In case an 'ip' command is used, the increment is specified as the second argument in parentheses.

1.5.3.3 Phase program position

Phase programs must be specified at the end of the pulse program after the "exit" statement (see the pulse program example in Table 1.1 at the beginning of this chapter). Any pulse program can contain up to 32 different phase programs (ph0-ph31).

1.5.3.4 Phase cycling

At the start of a pulse program, the first phase of each phase program is valid. The next phase becomes valid with the next scan or dummy scan. When the end of a phase program is reached, it starts from the beginning (*phase cycling*).

1.5.3.5 Phase pointer increment

The phase pointer in all phase programs is automatically incremented by the go statement. However, it is also possible to explicitly switch to the next phase as shown in the following example:

    p1:f2 ph8^
    p2:f2 ph8

p1 is executed with the currently active phase of ph8, then p2 is executed with the next phase in ph8. The caret (^) postfix in the first line, increments the phase pointer to the next phase in the list. This phase will become valid with the next pulse program statement that includes this phase program (note that this can be the same statement if it is included in a loop).

The following example is equivalent to the one above:

    p1:f2 ph8 ipp8
    p2:f2 ph8

Only in this case the statement ipp8 is used to increment the pointer in the phase program ph8. Please note that ipp8 is specified on the same line as p1 and therefore does not cause an extra delay between p1 and p2. The increment statements ipp0-ipp31 are available for the phase programs ph0-ph31. Increment statements can also be specified with a delay rather than a pulse. For example,

    d1 ipp7

moves the pointer to the next phase in ph7.

If explicit phase program manipulation is used in the pulse program, the phase program concerned will no longer be incremented with the go command.

The statements rpp0-rpp31 can be used to reset the phase program pointer to the first element. The statement zd automatically resets all phase program pointers to the first item, whereas the statement ze sets the pointer such that after DS dummy scans the pointer will be at the first element of each phase program. Phase programs that use the autoincrement feature or explicit incrementation with ipp are not incremented by the go statement at the end of a scan.

dpp0 - dpp31 can be used analogously to go back to the previous phase

program item.

1.5.3.6 Adding a constant to a phase program

You can change all phases in a phase program by a constant amount with the **:**r option. Each phase program ph0-ph31 has a constant assigned to it, PHCOR[0]-PHCOR[31]. These can be set from *eda*, or by entering *phcor0* etc. on the command line. For example, with ph8 = 0 1 2 3 and PHCOR[8]=2°, the phases of the pulse:

      (p1 ph8**:**r)**:**f2

are 2, 92, 182, 272 degrees. Without the **:**r option, the phase cycle of p1 would be 0, 90, 180, 270 degrees. The **:**r option can be used together with the caret postfix, e.g.:

      (p1 ph8^**:**r)**:**f2

1.5.3.7 Phase program arithmetic

Each of the phase programs ph0-ph31 has 3 associated statements:

      ip0-ip31, dp0-dp31, rp0-rp31.

They can also be used with an integer multiplier n:

      ip0*n - ip31*n, dp0*n - dp31*n.

Consider the phase programs ph3 = 0 2 2 0 and ph4 = (5) 0 1 2 3. The pulse program statement:

      20u ip3

increments all phases of ph3 by 90°. The next time that ph3 is encountered, its phase cycle will be "1 3 3 1". Likewise, the pulse program statement:

      20u ip4

increments all phases of ph4 by 360/5 degrees. The next time that ph4 is encountered in the pulse program, its phase cycle will be "(5) 1 2 3 4".

The statements dp0-dp31 decrement all phases of the associated phase program. The statements rp0-rp31 reset all phases of a phase program to their original values, i.e. to the values they had before the first ip0-ip31 or dp0-dp31.

The statements:

        6u ip3*2
        7.5u dp4*2

increment ph3 by 2*90=180° and decrement ph4 by 2*360/5=144°.

An increment/decrement phase program statement must always be specified behind a delay, which must be long enough for the increment/decrement to be calculated. The required time depends on the number of phases in the phase program and amounts to 1.5 msec per phase and channel.

1.5.3.8 Phase Program Modifications at Runtime

For AV and AV II spectrometers, the commands in this and the following section cause the pulse program to be executed from the TCU, whereas normal phase program commands are executed from the FCU. (Execution from the TCU makes the TCU performance slower. It can be forced for normal phase programs as well with the command 'phaseOnTcu' somewhere in the pulse program.) For AV III spectrometers, there is no such difference.

        (1) p1 ph=91.5
        (2) (d1 p21:sp2 ph=cnst30):f2
        (3) p1 ph1+ph2
        (4) p1 ph1+90
        (5) p1 ph=cnst30+90

In (1), a phase is set to a value given explicitly in degrees.

In (2), the phase is set from the parameter cnst30, which can be calculated in a relation at some other place in the pulse program before.

In (3), the phases of 2 phase programs are added together.

In (4), a constant offset is added to a phase program. This is especially useful in subroutines, where a phase program is defined in the main program and phases in the subroutine are set relative to this phase program.

In (5), the parameter cnst30 is used with an offset.

1.5.3.9 Calculation and Usage of Phase Programs at Runtime

There are 2 ways to calculate constants from phase programs and set

phases at runtime:

(1)

```
"cnst30=ph1+nsdone*90"
p1 ph=cnst30
```

(2)

```
"ph1=(nsdone%8)*45"
p1 ph1
```

In example (1), cnst30 is calculated, using a phase program and adding a variable amount to it depending on the current scan counter. cnst30 the is used some time later in the pulse program to set the phase of pulse p1.

In (2), the current value of phase program ph1 is overwritten with some value calculated from the scan counter. The pulse p1 will have this phase as long as no phase program manipulation command is executed between the two statements. Any such command will replace the current phase value with the value from the original phase program.

1.5.3.10 Runtime Changes of the Phase Program Increments

The ip statement can also be used to add increments other than the amounts defined in the definition of the phase program. This is done using the parameters CNST[0]-CNST[31] (which can have a positive or negative value). For example, the statement:

```
d11 ip1+cnst23
```

adds the value of CNST[23] to each phase of the phase program ph1.

A constant can also be defined in the pulse program. As such it is calculated at runtime. For example, the section:

```
"cnst23=d0*360/24;"
d11 ip1+cnst23
```

calculates a phase from the current value of d0 and then puts it into the parameter cnst23. Then it adds this value (in degrees) to each phase of the phase program ph1. Note that ip1+cnst23 works on the <u>original</u> phase program ph1 whereas ip1(*n)works on the <u>current</u> phase program ph1.

As an example, the next pulse program section increments the phase at

runtime depending on the number of scans done:

```
"cnst5 = 20"
2 d1
p1 ph1
6u ip1+cnst5 ; set the phase program to the original values + cnst5 °
"cnst5= nsdone*30"
go =2 ph31
ph1 = 0 2 2 0 1 3 3 1
```

1.5.3.11 Phase setting without executing a pulse

Phases can be set after pulses or delays. TOPSPIN allows you set the phase for a particular spectrometer channel without executing a pulse. In that case, you must specify a phase program behind a delay. Example:

```
(d1 ph1):f3
(p11:spf1):f3
```

Note that on AV spectrometers there is no frequency while there is no pulse. This kind of phase setting makes sense only if there is no time to set the phase during the pulse (e.g. for ultrafast shape pulses).

1.5.3.12 Definition of phase programs using list syntax

Instead of setting up ph0-ph31 at the end of the pulse program, a phase program may also be defined by a list definition, which must then occur before the actual start of the pulse program (beginning with ze):

```
define list<phase> PhList1={0.0 180.0 90.0 270.0}
```

This statement defines the phase program *PhList1* with phase values of 0°, 180°, 90° and 270°. Note that in contrast to the previously described definitions of phase programs, all angles are written in degree in this syntax. Instead of initializing the phase program directly with {}-brackets, you may also specify the file name of a phase program or the variable PHLIST which contains such a filename, both in angle brackets. Examples,

```
define list<phase> PhList2=<myphaseprogram>
define list<phase> PhList3=<$PHLIST>
```

In both cases, the file that contains the phase program can be created with the command ***edlist phase***.

Phase setting from user-defined phase programs is done in exactly the same way as with the standard phase programs by specifying the phase program after a pulse statement.

After initialization, the current value of a user-defined phase program is its first entry. You can access other entries by using the list operations .inc, .dec, or .res to increment, decrement, or to reset the index. By using the caret postfix operator (^) you can combine phase setting with an increment operation, as with other list types or with the standard phase programs. However, in contrast to other list types, you can neither retrieve a particular entry using the []-bracket notation, nor set the index directly by assigning to *PhList1.idx.* Furthermore, no equivalents to the ipX, dpX, and rpX statements available with the standard phase programs ph0-ph31 exist for user-defined phase programs.

Note that user-defined phase program names may consist of up to 19 characters, but only the first 15 are interpreted. Up to 32 user-defined phase programs may be defined in a single pulse program. It is furthermore possible to define the standard phase programs ph0 to ph31 with the above syntax. In this case the phase program base (used for the ip0-ip31, and dp0-dp31 statements) is implicitly 65536 (equivalent to 16 bits). Using an ipX command on a standard phase program defined with the above syntax will shift all of its phase entries by $360°/65536 \approx 0,006°$. After 65536 ipX statements, the phase program entries would have returned to their initial values. To make a 90° phase increments use ipX*16384.

1.5.4 Pulse power and shape

1.5.4.1 Rectangular pulses

A *rectangular* pulse has a constant power while it is executed. It is set to the current power of the spectrometer channel on which the pulse is executed. The default power for channel f1, f2, ... , f8 is PL[1], PL[2], .., PL[8]. Here, PL is an acquisition parameter that consists of 32 elements PL[0] - PL[31]. It can be set from *eda* or by entering *pl0*, *pl1*, etc. on the command line. You can set the power for a particular channel with the statements pl0-pl31. For example:

        d1 pl5**:**f2

sets the transmitter power for channel f2 to the value given by PL[5]. Any pulse executed on this channel will then get the frequency SFO2 and the power PL[5]. The pl0-pl31 statements must be written behind a delay. The power setting occurs within this delay, which must be at least 0.2 msec.

The power can be set not only from these parameters but also from constants, from the parameters SP0..31 and directly as a number:

```
d1 pl=cnst23:f1
d1 pl=sp7:f1
d1 pl=3:f1
```

1.5.4.2 Power lists

In addition to the above possibilities, you can use user defined power lists on Avance spectrometers. A user defined power list is defined and initialized in a single define statement, e.g.:

```
define list<power> pwl = { -6.0 -3.0 0 }
```

The define list<power> key is followed by the symbolic name, under which the list can be accessed in the pulse program. The name is followed by an equal sign and an initialization clause, which is a list of high power values, in dB, enclosed in braces. Entries must be separated by white spaces.

You can access a power list by specifying its name, e.g.:

```
d1 pwl:f1
```

sets the power of channel f1 to -6.0 dB, when it is used for the first time. You can move the pointer within a power list with the increment, decrement and reset postfix operators .inc, .dec, .res. For example, you can switch to the next entry of the above list with the statement:

```
pwl.inc
```

Alternatively, you can use the caret (^) operator to set the power and increment the list pointer within one statement. For example, the statement:

```
d1 pwl^:f1
```

is equivalent to:

```
d1 pwl:f1 pwl.inc
```

You can also access the list index in a relation, appending **.**idx to the symbolic name, e.g:

> "pwl**.**idx = pwl**.**idx + 1"

The above expression is equivalent to:

> pwl**.**inc

Furthermore it is possible to access a certain list element by specifying its number in square brackets, for example:

> pwl[2]

Note that list indices start with 0. All index calculations are performed modulo the length of the list. In the above example pwl[3] = pwl[0] = -6.0.

Note that index manipulations are executed at the end of the duration. This means, for example, that the statement:

> d1 pwl^**:**f1 pwl**:**f2

will set both the f1 and f2 channel to the same power level.

As an alternative to initializing a list, you can specify a list file in angle brackets, e.g.:

> define list<power> fromfile = <pwlist>

Such a file can be created or modified with the command **_edlist va_**. Instead of a filename you can also specify $VALIST, for example:

> define list<power> fromva = <$VALIST>

In this case, the filename is defined by the VALIST acquisition parameter.

Note that the number of user defined lists is limited to 32 for each list type. The length of the name is arbitrary, but only the first 7 characters are interpreted.

The following example shows the use of an initialized power list:

Example:

> define list<power> pwl = { 10 30 50 70 }
> ze
>
> 1 d1 pwl:f1 pwl.inc   ; set power on f1 to 10dB, incr.

```
        pointer
          d1 pwl:f2 pwl.dec              ; set power on f2 to 30dB, decr.
        pointer
          d1 pwl[2]:f3                   ; set power on f2 to 50dB
          "pwl.idx = pwl.idx + 3"        ; set the pointer to 0 to 3
          d1 pwl^:f4                     ; set power on f4 to 70dB, incr.
        pointer
            (p1):f1 (p2):f2 (p3):f3 (p4):f4
          go=1
        exit
```

1.5.4.3 Shaped pulses

A *shaped* pulse changes its amplitude (and possibly phase) in regular time intervals while it is executing. The pulse *shape* is a sequence of numbers (stored in a file, see below) describing the amplitude and phase values which are active during each time interval. The interval length is automatically calculated by dividing the pulse duration by the number of amplitude values in the shape file. If this is less than the minimum duration, an error message is displayed which tells you what is the minimum pulse duration for this shaped pulse.

The next 3 examples generate shaped pulses:

```
        (10mp:sp2 ph7):f1
        (p1:sp1 ph8):f2
        (p30d1H*3.33:sp3 ph9):f3
```

The pulse durations are 10 millisec, P[1], and p30d1H*3.33, respectively. The pulses are executed on the frequency channels f1, f2, and f3 (i.e. the pulse frequencies are SFO1, SFO2, and SFO3), respectively. The pulse shape characteristics are described by the entries 2, 1, and 3 (corresponding to :sp2, :sp1, and :sp3) of the *shaped pulse parameter table*. This table is displayed when you click the SHAPE button within *eda*. The table has 32 entries with the indices 0-31. You may use the statements :sp0 - :sp31 to refer to the entries 0-31, respectively. As you can see from the examples, a phase program can be appended to a shaped pulse in the same way it can be appended to a rectangular pulse. The current phase of the phase program is added to the phase of each component of the shaped pulse.

Note that the statement:

      (vp:sp4 ph10):f4

is <u>incorrect</u> because shaped pulses with vp are not supported.

Each entry of the shaped pulse parameter table has 4 parameters assigned to it: a *power value*, an *offset*, a *file name* and a phase *alignment*.

File name
The name of a shape file. A shape file can be generated with the command **st**. or from the Shape Tool interface (command **stdisp**). Shape files are stored on disk in the so called JCAMP format. They reside in the directory:

   $XWINNMRHOME/exp/stan/nmr/lists/wave/

After its header, a shape file contains a list of entries, one entry for each pulse shape interval. Each entry consists of an amplitude value (in percent) and a phase value (in degree). The amplitude value defines the percentage of the absolute power value (see below).

Offset frequency [Hz]
The shape offset frequency allows you to shift the frequency of the shaped pulse by a certain amount (in Hertz). This shift is realized by applying phase changes during the shaped pulse's time intervals. In this way, phase coherency of the frequency is maintained.

Power value [dB]
This is the absolute power value of the pulse shape. The actual power value of a particular shape interval is the absolute power value multiplied by the relative power value of that interval, as specified in the shape file. The power of the shape is set in the interval before the start of the shape and reset to the default power setting of the channel (in this case PL[1] for channel F1) after the shape. The power setting which was actual before the shape is lost. For this reason it is not possible to execute pulses immediately before and after the shape, because there must be delays in which the power setting is done. (For AV instruments these delays must be 3ms before and after the shape and 4ms between two shapes, for AV III instruments no such extra delay is required, but the minimum length of a shape segment which is normally 25ns can be executed only if there is no power setting and phase setting associated with this shape.)

      d20 pl9:f1   ; set power on channel f1 to PL[9]
      p1:sp0:f1   ; shaped pulse with abs. power

```
        SP[0]
        d11
        p2:f1                                   ; rectangular pulse with power PL[1]
```

Rather than using power values specified in SHAPE, you can also use the power value that is currently active on the channel that you use. You can do that with the (currentpower) modifier of the sp statement as shown the following example:

```
        d20 pl9:f1                     ; set power on channel f1 to PL[9]
        p1:sp0(currentpower):f1        ; shaped pulse with abs. power PL[9]
        p2:f1                          ; rectangular pulse with power PL[9]
```

If, in this example, the value of PL[9] is very different from the value of SP[1], the pulse shape may be compressed. The reason for this is that the CORTAB correction table for SP[1] is applied rather than for PL[9]. The advantage of this method is that you can use pulses immediately before and after the shape.

You can access the SHAPE table entries from *eda*. However, you can also set the entries from the command line. For example, *spnam5* allows you to set the file name of entry 5, *spoffs2* sets the frequency offset of entry 2 and *sp15* sets the absolute power value of entry 15.

Phase alignment

Shapes with frequency offsets do vary the phase in order to efficiate the frequency shift. By this variation the total phase of the shape is affected as well. The parameter SPOAL[0..31] determines whether the phase is aligned relative to the start or the end of the pulse. SPOAL has a range of 0 to 1. If SPOAL = 0, the relative phase shift is 0 at the beginning of the pulse whereas it is determined by the frequency offset SPOFFS and the pulse length at the end of the pulse. If SPOAL = 1 the relative phase shift is 0 at the end of the pulse.

Using shapes with variable pulse length

A shaped pulse can be used in connection with a variable duration. For example, the pulse p1 has a duration P[1] and can be varied with statements like ipu1 or "p1=p1+0.5m".

For a shape consisting of 1000 points the following restrictions apply (not for AV III instruments):

- the minimum execution length is 1000*7*50 ns = 200 msec.
- the increment must be a multiple of 50*1000 ns. Any other increment values might result in spikes after the shape.

When a shape is specified too short or too long, an error message will be printed and the shape will be used with the previous settings!

The length of a shaped pulse can be varied with a statement like:

    ipu1

or with a relation like:

    "p1 = p1 + 0.5m"

In both cases, the variation of a shape pulse length takes 4 msec per channel.

Note that varying the length of a shape with non-zero-offset-frequency will change the offset frequency, as the frequency shift is obtained via phase shifting. This phase shift won't be recalculated during execution, so the offset will be changed inverse proportional to the duration. (Doubling the duration means cutting the offset in half). An warning will be printed, when you change the duration of a shape with offset.

1.5.4.4 Fast Shapes

(AV and AV II instruments only.) Regular pulse shapes as described above need a short delay before and after the pulse of ~4 msec. On Avance-AQS, you can also generate the so-called fast shapes. They do not require this delay so fast shaped pulses can be executed consecutively in a loop or they can be executed right before or right after a rectangular pulse. Fast shape pulses and can be executed with the options :spf0 - :spf31. They differ from normal shapes in the following respects:

- They do not change the power setting but use the current setting.
- The minimum time for each interval is 350 nsec whereas for normal shapes it is between 50 and 100 nsec. If this limit is violated, the pulse programs will stop with the error message: "AQNEXT while FIFO busy".
- The timing of the shape cannot be changed during pulse program execution.

- The total time of the entire shape must be exactly the time for one inter-val times the number of intervals in the shape pulse, where the timing resolution of the time for the intervals is 50 ns (whereas the time resolu-tion for normal shapes is 12.5 ns).

Fast shapes are typically used for solid states experiments.

1.5.4.5 Shape lists

Instead of a single shape, one can also use different shapes from a shape list and toggle through the list with the list increment command.

define list<shape> shl=<wavelist>

This statement defines a new object called shl which represents a shape list and can be used in the same way as the normal shapes sp0-sp31. With the command

shl.inc

the next item from the shape list becomes active.

A shape list file has a format similar to the shape parameter list in the editor where each entry consists of a line containing 4 items:

#Power[dB]	Offset[Hz]	Offset alignment	Shape file name
1.0	0.0	0.5	Gauss
...			

1.5.4.6 Amplitude Lists

On AV you can define amplitude lists in a pulse program, for example:

define list<amplitude> am1={70}

The amplitude values represent the percentage of the power of a rectangu-lar pulse. The above list is interpreted by a statement like:

d11 am1:f1

which reduces the power on the f1 channel to 70% of PL[1] (assuming it

was at its default value PL[1]). All rectangular pulses on f1 will then be executed with this reduced power. A statement like:

     d12 pl1**:**f1

will reset the power on channel f1 to 100% of PL[1]. Furthermore, a shape pulse like

     p11:sp1:f1 ph1

sets the power on f1 to either

*   100% of PL[1] on AV or AV II systems
*   to the power SP[1] and the last amplitude of the shape after it has finished.

An example of a pulse program segment using an amplitude list is:

     define list<amplitude> am1={70}

     p1 ph1   ; rectangular pulse on f1 with power PL[1]
     d11 am1:f1   ; set the power on f1 to 70% of PL[1]
     p1 ph2   ; rectangular pulse on f1 with 70% of PL[1]
     ...

Amplitudes can be set also with the following statements;

     d11 amp=amp1:f1   ; set the amplitude on f1 to the value AMP[1]
     d11 amp=cnst2:f1   ; set the amplitude on f1 to the value CNST[2]
     d11 amp=70:f1   ; set the amplitude on f1 to 70%

1.6 Delay generation

Table 1.6 shows the available types of statements for the generation of delays. The duration of a delay corresponds to the name of the delay statement.

1.6.1 <u>d0</u>-<u>d31</u>

The statement:

`d0, d1, ... , d31`	Generate a delay whose duration is taken from the acquisition parameter D[0], ..., D[31], respectively.
`d0:r, ... d31:r`	Generate a delay whose duration is taken from the acquisition parameter D[0], ..., D[31] and which is randomly varied. The maximum variation (in percent) is defined by the acquisition parameter V9.
`3.5u, 10m, 0.1s`	Generate a delay of fixed length: u = μsec , m = msec, s = sec.
`compensationTime`	Generate a delay whose name is defined with a `define delay` statement, and whose duration is defined by an expression.
`vd`	Generate a delay whose duration is taken from in a delay list.
`de1, de, depa, derx, deadc`	Generate a delay of length DE1, DE, DEPA, DERX, DEADC, respectively.
`dw, dwov`	Generate a delay of length DW, DWOV.
`aq`	Generate a delay of length AQ.
`acqt0`	Determines 0-point of FID

Table 1.6 Delay generation statements

> d0

executes a delay of width D[0], where D[0] is an acquisition parameter. It is set from *eda*, or by typing *d0* on the command line. Likewise, the statement:

> d1

executes a delay of width D[1].

1.6.2 Random delays

The statement:

> d0:r

executes a delay of width D[0] which is varied randomly. The parameter V9 specifies, in percent, the maximum amount which is added to or subtracted

from D[0]. As such, the effective delay varies between 0 and 2*D0. It can be set from *eda*, or by typing *v9* on the command line.

Please note that the *gs* command ignores the :r option.

1.6.3 Fixed length delays

The statement:

    10m

executes a delay of 10 msec (called a *fixed delay* because its duration cannot be manipulated, see below). The duration must be followed by u, m, or s. These units indicate microseconds, milliseconds, and seconds, respectively.

1.6.4 User defined delays

The statement:

    define delay compTime

defines compTime to be a delay statement and the statement:

    "compTime=d1*0.33".

is the expression that defines its duration. Note that the double-quote characters (") are obligatory.

With the above statements, the statement:

    compTime

executes a delay whose name is defined in the pulse program, and whose duration is determined by an arithmetic expression. The define statement must be inserted somewhere at the beginning of the pulse program, before the actual pulse sequence.The defining expression must also occur before the actual pulse sequence. It is evaluated at compile time of the pulse program, not at run time.

Names for user defined delays must consist of alphanumeric characters, and the first character must be an alphabetic character. The maximum length of the name is 11 characters. Caution, do not use any of the reserved words like ,adc', ,go', ,pulse' etc. as a delay name.

1.6.5 Variable list delays (obsolete)

The statement:

> vd

executes a delay whose duration is given by the current value of a variable delay list. A delay list is a text file that contains one delay per line. Delay lists are set up with the command **edlist vd** (described in the Acquisition Reference manual). The statement vd uses the list file defined by the acquisition parameter VDLIST. When the pulse program is started, the first duration in the list is used. The pulse program statement ivd can be used to move the list pointer to the next duration. If the end of the list is encountered, the pointer is reset to the beginning. The statement ivd must be specified behind a delay, for example:

> d1 ivd
> 0.1u ivd

The length of the delay is irrelevant, any value is allowed.

It is also possible set the list position with an equation. Example:

> "vdidx=5"
> vd

Here, vd will execute a delay whose duration is selected from position 5 of the delay list. To the right of the equal sign any dimensionless expression is allowed. This may contain parameters from Table 1.3.

1.6.6 User Defined Delay Lists

As an alternative to using the vd statement, a list of delays can also be specified with a define statement in the following way:

> define list<delay> Dlist = { 0.1 0.2 0.3 }

This statement defines the delay list Dlist with the values 0.1sec, 0.2sec and 0.3sec. Instead of delay values, you can specify a list filename in the defined statement. There are two way of doing this: you can specify the actual filename or $VDLIST, both in <>. In the latter case, the file defined by the acquisition parameter VDLIST is used. For example:

> define list<delay> D2list = <mydelaylist>
> define list<delay> D3list = <$VDLIST>

In both cases, the file an be created or modified with the command ***edlist vd***.

In a pulse program that contains the statements above, the statement:

D1list

executes a delay of 0.1seconds the first time it is invoked. In order to access different list entries, the list index can be incremented by adding **.**inc, decremented by adding **.**dec or reset by adding **.**res. Index operations are performed modulo the length of the list, i.e. when the pointer reaches the last entry of a list, the next increment will move it to the first entry. Furthermore, a particular list entry can be specified as an argument, in squared brackets, to the list name. For example, the statement:

D1list[1]

executes a delay of 0.2 seconds. Note that the index runs from 0 to n-1, where n is the number of list entries.

Lists can also be executed and incremented with one statement, using the caret postfix operator. For example, the statement:

D1list^

is equivalent to:

D1list D1list.inc

Finally, you can set the index with an arithmetic expression within double quotes using **.**idx postfix. The following example shows the usage of an initialized delay list:

```
define list<delay> locallist = {0.1 0.2 0.3 0.4}

locallist locallist.inc        ; delay of 0.1s, set index from 0 to 1
locallist locallist.res        ; delay of 0.2s, set index to 0
locallist[2]                   ; delay of 0.3s
locallist locallist.dec        ; delay of 0.1s, set index from 0 to 3
locallist                      ; delay of 0.4s
"locallist.idx = 3"            ; set index to 3
locallist^                     ; delay of 0.4s, set index from 3 to 0
locallist                      ; delay of 0.1s
```

Note that there are two restrictions on the multiple use of delay lists within

the same line:

- Index operations take effect from the next line on
- Furthermore, you cannot access two different entries of the same list in one pulse program line as illustrated in the following example:

```
locallist^ locallist          ; executes the first list entry (0.1s)
twice
locallist                     ; increment takes effect now (0.2s
delay)
locallist[2] locallist[3]     ; executes the third entry (0.4s) twice
```

Note that names for user defined items may consist of up to 19 characters but only the 7 first are interpreted: i.e Delaylist1 and Delaylist2 are allowed names but would address the same symbol.

1.6.7 Special Purpose Delays

These are the delay statements de1, depa, derx, deadc, de as listed in Table 1.6. They are used in pulse programs in which the acquisition is started with the adc statement rather than with go=label. Implicitly they are used in the go macro as well and can be set in the edscon table or explicitly within the pulse program. dw and aq are determined by setting the sweep width and cannot be redefined within the pulse program.

The delay acqt0 is a delay which is not used by the pulse program compiler but in connection with the *baseopt* option of DIGMOD. It serves to determine the point where t=0 for the FID. This point is for a simple zg program somewhere in the middle of the excitation pulse. One therefore defines this delay as

```
"acqt0=-p1*3.14159/2"
```

The linear prediction software takes this value to reconstruct the part of the FID which could not be measured.

1.6.8 Manipulating Delays: The Operator *

A delay can be manipulated by the "*" operator. Examples of allowed statements are:

```
d1*1.5
compensationTime*3.33
```

<div style="text-align: right;">

d3*oneThird
vd*3

</div>

The * operator must be specified behind the delay statement, not before. *oneThird* is the name of a macro that must be defined at the beginning of the pulse program with a statement like #define oneThird 0.33. Note that a statement like 10m*0.33 would be incorrect, since 10m is a fixed delay.

1.6.9 Manipulating Delays: Changing <u>d0</u>-<u>d63</u> by a Constant Value

The delays executed by d0-d63 can be incremented or decremented according to the acquisition parameters IN[0]-IN[63]. These parameters contain a duration (in seconds). The pulse program statements id0-id63 add IN[0]-IN[63] to the current value of d0-d63, respectively. Likewise, dd0-dd63 subtract IN[0]-IN[63] from the current value of d0-d63. The statements rd0-rd63 reset d0-d63 to their original value, i.e. to the values of the parameters D[0]-D[63]. The statements presented in this paragraph must be specified behind a delay of any length. Examples:

d1 id3
0.1u dd0
d1 rd0

In Bruker pulse programs, D[0] and D10 are used as incrementable delays for 2D and 3D experiments, IN0 and IN10 are the respective increments which are used to calculate the sweep widths SW(F1) and SW(F2), respectively (see the description of IN0, IN10 in the Acquisition Reference manual).

1.6.10 Manipulating Delays: Redefining <u>d0</u>-<u>d63</u>

The duration of the d0-d63 statements is normally given by the parameters D[0]-D[63]. However, you can overwrite these values in the pulse program using an expression in C language syntax. The following examples show some of the possibilities:

"d13=3s + aq - dw*10"
"d13=d13 + (p1*3.5 + d2/5.7)*td"

The result of such an expression must have a time dimension. You can therefore include acquisition parameters such as pulses, fixed pulses, delays, fixed delays, acquisition time AQ, dwell time DW etc. within the

expression. Furthermore, you can include parameters without a dimension such as the time domain size TD. The complete list is shown in Table 1.3. An expression must be double-quoted (" "). It can be inserted anywhere in the pulse program, as long as it occurs before the delay statement that uses the expression (d13 in our example). Please note that the second expression in the example above assigns a new value to d13 each time the expression is encountered, for example in a loop.

1.6.11 Manipulating the Durations of User Defined Delays

You can define your own delay statements using a define statement like:

> define delay compensationTime

at the beginning of the pulse program. This delay is executed by the statement:

> compensationTime.

The delay length must be defined with a statement like:

> "compensationTime=d1*0.33".

For such an expression the same rules apply as for the manipulation of d0-d31, described in the previous section.

Note: The defining expression of a user defined delay must occur before the start of the actual pulse sequence. It is evaluated at compile time of the pulse program, not at run time.

1.6.12 *larger* and *random*

In order to avoid complicated expressions for the assignment of delays and pulses, the comparison of two delays and can be made like this:

> define delay delta
> "delta=larger(p4,d2)"

In this expression the length of p4 and d2 are compared, and the delay delta will become equal to the longer one.

In order to randomize a delay or a pulse only at a certain point of the program, one can use the following:

> "p4=random(p1,20)"

which will assign p4 the value of p1*(100+20*R)/100, where R is a random number in the range of -1 to +1. This can be used, where the pulse p4 should be changed not each time it is used, but for instance only after ns scans. (The usage of p4:r within the pulse program randomizes the pulse each time when it occurs).

1.7 Simultaneous Pulses and Delays

1.7.1 Rules

The following rules apply in pulse programs:

1. Pulses and delays specified on subsequent lines are executed sequentially.

2. Pulses and delays which are specified on the same line, and which are enclosed in the same set of parentheses or without parenthesis are executed sequentially. Such a sequence is called *pulse train* in the following.

3. Pulse trains on the same line are executed simultaneously. The first item within a pulse train is started at the same time as the first item in any other pulse train. You can specify an arbitrary number of sets of parentheses on a line.

4. Pulse trains on different lines which are enclosed by an extra set of parentheses are executed simultaneously.

1.7.2 Examples

1.7.2.1 Rule 1

The pulse program section:

```
(p1 ph1):f1
100u
(p2 ph2):f2
```

executes a pulse on channel f1, followed by a delay, followed by a pulse on channel f2 (Figure 1.1).
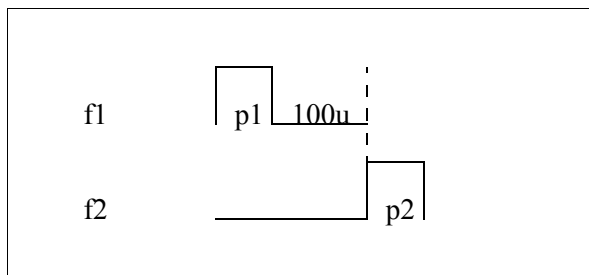
Figure 1.1 Rules 1 and 2: An example

1.7.2.2 **Rule 2**

The pulse program section:

    (p1 ph1 100u):f1
    (p2 ph2):f2

executes a pulse on channel f1, followed by a delay, followed by a pulse on channel f2 (Figure 1.1).

1.7.2.3 **Rule 3**

The pulse program section:

    (p1 ph1):f1 (100u)
    (p2 ph2):f2

executes a pulse on channel f1.

At the same time, the 100 msec delay begins, since it is enclosed in a separate set of parentheses. The pulse on channel f2 is not executed before either p1 or 100u have passed, whichever is longer (Figure 1.1)..

The following example is a typical section of a DEPT pulse program:

    (p4 ph2):f2 (p1 ph4 d2):f1
    (p0 ph3):f2 (p2 ph5):f1

The pulses p4 and p1 begin at the same time, p4 on channel f2 and p1 on channel f1. The pulses p0 and p2 start simultaneously, but not before the sequence with the longest duration of the previous line has finished (Figure 1.3).
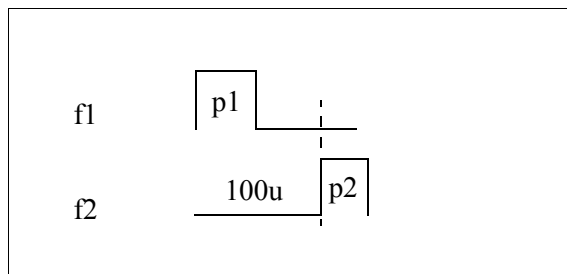
Figure 1.2 Rule 3: example 1
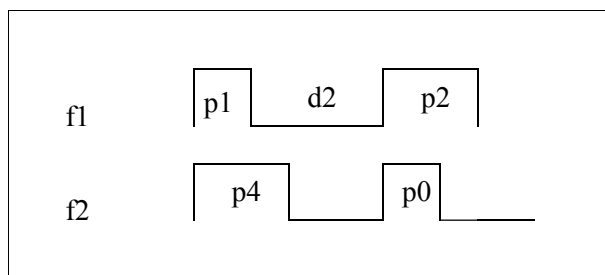
Figure 1.3 Rule 3: DEPT example

The following 2 lines have been extracted from the *colocqf* Bruker pulse program.

    (d6) (d0 p4 ph2):f2 (d0 p2 ph4):f1
    (p3 ph3):f2 (p1 ph5):f1

We have three sets of parentheses in this case. The first item in each set of parenthesis, i.e. d6 and d0, start at the same time. After d0, p4 on channel f2 and p2 on channel f1 start simultaneously. Assuming that d6 is larger than d0+p4 and d0+p2, the second line is executed after d6 has finished.

A final example for rule 3 is a line from the *hncocagp3d* Bruker pulse program:

    (p13:sp4 ph1):f2 (p21 ph1):f3

The shaped pulse p13 on channel f2 is started simultaneously with the rectangular pulse p21 on channel f3.

1.7.2.4 Rule 4:

The example in the previous section can be rewritten according to this rule

```
(
  (d6)
  (d0 p4 ph2):f2
  (d0 p2 ph4):f1
)
(p3 ph3):f2 (p1 ph5):f1
```

It still produces the same pulse sequence.

1.7.3 Pulse Train Alignment

Pulse trains written in the style of rule 4 can be aligned in different ways.

1.7.3.1 Global Alignment

There are three global alignment possibilities for the pulse trains: left alignment (lalign) is the default, right alignment (ralign) will arrange the pulse sequences such that all of them end at the same time, and center alignment (center) will start the pulse trains in such a way that they are centered according to the mid-point of the longest of them. The global alignment must be specified after the first opening bracket:

```
(center
  (d6)
  (d0 p4 ph2):f2
  (d0 p2 ph4):f1
)
```

1.7.3.2 Individual Alignment

Single pulse trains can be aligned individually as well. In this case, the first pulse train in a sequence must be defined as the reference (refalign):

```
(
  refalign (d0 p1 ph1 d0):f1
  center (p2 ph2):f2
  ralign (p3 ph4):f3
)
```

Pulse train 3 is now right-aligned relative to pulse train 1, pulse train 2 is centered relative to pulse train 1. From this piece of code several situations may result which are not obvious but best can be shown graphically: only in 2 of the 6 possible cases the sequence begins with the reference pulse train.
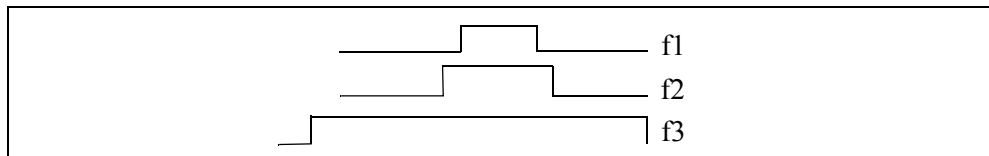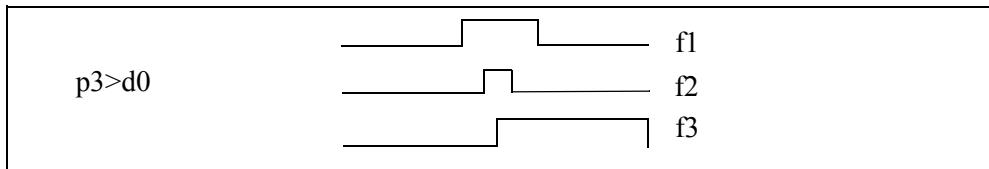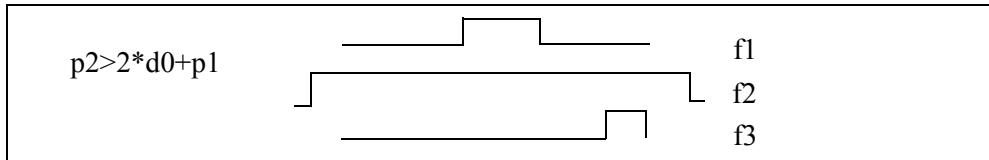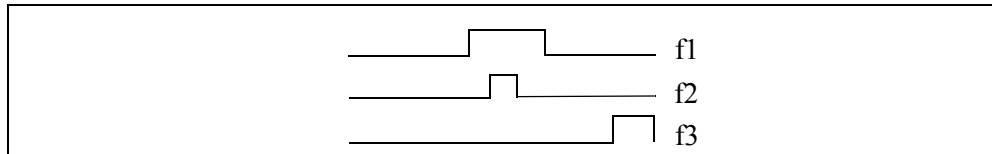
If the length of individual pulse trains change during pulse program evolution, the alignment conditions will still be true.

Chapter 2

Decoupling

2.1 Decoupling

2.1.1 Decoupling Statements

Table 1.6 shows the available types of decoupling statements. Composite pulse decoupling is discussed in more detail in the next section of this chapter.

cw	continuous wave decoupling
hd	homodecoupling
cpds1, .. ,cpds8	composite pulse decoupling with CPD sequence 1, ..., 8, synchronous mode
cpd1, .. ,cpd8	composite pulse decoupling with CPD sequence 1, ..., 8, asynchronous mode
cpdhd1,.. cpdhd8	homodecoupling using CPD seq. 1,...
do	switch decoupling off

Table 2.1 Decoupling statements

Each pulse program line can contain one (and only one) decoupling statement. For example, the line:

    d1 cw:f1

turns on cw-decoupling on channel f1 at the beginning of delay d1. The line:

    go=2 cpds1:f2

turns on composite pulse decoupling on channel f2 at the start of the FID detection.

Decoupling statements are allowed in pulse program lines that contain a delay statement or the go statement, but not in lines with pulses, expressions or any lines with any of the statements adc, rcyc, lo, if or goto.

Once decoupling is turned on, it remains on, until it is explicitly turned off with do. For example:

    0.1u do:f1

turns decoupling off on channel f1.

cpdhd1..8 is used for homodecoupling during the acquisition for AV III systems. It uses the cpd programs CPDPRG1..8 but chopped in the HD manner. The decoupling is turned off after the scan automatically and needs no do statement:

    go=2 ph31 cpdhd1:f2

2.1.2 Decoupling Frequency

The decoupling frequency is selected by specifying the spectrometer channel behind the decoupling statement. In contrast to pulse statements, decoupling statements must be specified with! For example:

    d1 cw:f2

turns on cw decoupling on channel f2, i.e. with the frequency SFO2. This syntax is the same as used for selecting pulse frequencies (see the chapter 1.5.2). The statement:

    0.1u cpds1:f3

turns on the composite decoupling sequence 1 on channel f3, i.e. with the

frequency SFO3. The statement:

    3m do:f3

terminates decoupling on channel f3 at the beginning of the 3 msec delay.

2.1.3 Decoupling Phase

The relative phase of the decoupling frequency can be controlled using a phase program. This is equivalent to controlling the phases of pulses (see chapter 1.5.3). Examples:

    (d1 cpds1 ph2):f3
    0.1u (cw ph1):f2

Note that phase cycling (see chapter 1.5.3.4) is applied to phase programs specified behind decoupling statements in the same way that phase programs are specified with pulses. A simple example demonstrating this feature is the pulse program section:

    1m (cw ph1):f2
    d1 do:f2

which is equivalent to:

    (1mp ph1):f2
    d1

A 1 millisecond pulse is executed on channel f2, followed by a delay d1. Its phase is cycled according to phase program ph1.

2.2 Composite Pulse Decoupling (CPD)

2.2.1 General

Composite pulse decoupling, as opposed to cw and hd decoupling, offers a large degree of freedom to set up your own decoupling pulse sequences. Up to 8 different CPD sequences can be used in a pulse program. For example, the line:

    d1 (cpds1 ph2):f3 (cpds2 ph4):f2

starts, at the beginning of duration d1, CPD sequence 1 on channel f3 and, simultaneously, CPD sequence 2 on channel f2. CPD sequence 1 is

obtained from a text file defined by the acquisition parameter CPDPRG1. Likewise, CPD sequence 2 is obtained from a text file defined by the acquisition parameter CPDPRG2, etc. A CPD sequence (= CPD program) can be a Bruker delivered sequence like WALTZ16, GARP or BB or it can be a user defined sequence. CPD sequences can be set up with the command **edcpd** (as described in the Acquisition Reference manual). Table 2.2 shows the statements available to start a CPD sequence; and Table 2.3

`cpds1, ... ,cpds8`	Start decoupling using the CPD program CPDPRG1, ... , CPDPRG8. The decoupling sequence will start at line 1.
`cpd1, ... ,cpd8`	Like `cpds1-cpds8`, however, the decoupling sequence will continue from the line where it was stopped using `do`.
`:f1, ..., :f8`	Channel selector. To be appended to the `cpd` statements.
`cpdngs1, .. ,cpdngs8` `cpdng1, ... ,cpdng8`	Same as the `cpd(s)` statements above, except that the transmitter gate for the specified channel will not be opened. Gating is controlled by the main pulse program, and can be tailored by the user.

Table 2.2 Available `cpd` statements

shows the statements available to build a CPD sequence.

2.2.2 Syntax of CPD Sequences

The syntax of CPD sequences is demonstrated by examples. Table 2.4 shows the realization of Broadband and Garp decoupling with CPD sequences. Each sequence is an infinite loop as indicated by the last statement:

jump to 1

As in pulse programs, the pulse width in CPD programs can be specified as a *fixed pulse*, (e.g. 850up) or with the statements p0-p31. The Garp

p0, ... , p31 10up, 5mp, 2.5sp pcpd1, ... , pcpd8	Generate pulses with durations P[0], ... , P[31]. Generate pulses in micro-, milli-, and seconds Generate a pulse with duration according to PCPD[1], ... , PCPD[8], depending on the channel where the CPD sequence is executed (use **eda** to set PCPD).
d0, ... , d31 10u, 5m, 2.5s	Generate delays with durations D0, ... , D31. Generate delays in micro-, milli-, and seconds.
*3.5 :135.5	Multiplier. Can be appended to p0-p31 or d0-d31. Phase in degrees. Can be appended to pulses.
:sp0, ... , :sp31	Shaped pulse selectors. Can be appended to pulses.

pl=
pl=5
pl=sp13
pl=pl25
	Power specifier (see example in Table 2.5):
	   in dB
	   according to shaped pulse parameters SP[0]-[15]
	   according to PL[0]-[15]

fq= fq=2357 fq=cnst25 fq=fq2	Frequency change in Hz (relative to SFO1 for channel 1, SFO2 for 2...) from the parameters CNST[0]-[31] from the frequency list specified in FQ2LIST
;	Begin of a comment (until end of line)
lo to *label* times *n* jump to *label*	Loop to *label n* times Branch to *label*. Usually the last statement.
#addphase #setphase	Special phase control statements

Table 2.3 statements available to build CPD sequences

sequence shows the usage of the lo to statement.

The Garp sequence, as well as the sequences in Table 2.5, make use of the statement pcpd to generate pulses. This enables the execution of the same sequence for different nuclei on different channels. For example, when executed on channel f2 (f3), the pulse duration of pcpd is given by the parameter PCPD[2] and PCPD[3], respectively. This allows you to specify the 90° pulse width for two different nuclei in PCPD[2] and PCPD[3], and decouple both nuclei within the same pulse program using the same CPD program.

Table 2.5 shows two CPD sequences based on shaped pulses. Shapes are specified in the same way they are specified in pulse programs using the :sp0, ... , :sp31 pulse selector options. The examples demonstrate the order in which duration multiplier, shape selector and phase must be specified.

The sequences in Table 2.4 and Table 2.5 do not contain a power setting

```
1  90up:0            1  pcpd*0.339:0
   160up:180            pcpd*0.613:180
   240up:0             pcpd*2.864:0
   ........            pcpd*2.981:180
   570up:0             pcpd*0.770:0
   680up:180           .......
   810up:0             pcpd*0.593:0
   960up:180          lo to 1 times 2
   1140up:0         2  pcpd*0.339:180
   1000up:180          pcpd*0.613:0
   850up:0             .......
   710up:180           pcpd*2.843:180
   .........           pcpd*0.729:0
   200up:0             pcpd*0.593:180
   110up:180          lo to 2 times 2
jump to 1           jump to 1
```

Table 2.4 Broadband and GARP CPD sequences

statement. Therefore, the current power setting of the main pulse program for the respective channel is valid.

cpdngs is used for sequences which do not need the transmitter. For instance the dwell time can be generated in this way (see pulse program *zgadc* in the Bruker library). Another field of application is broadband hd with AV II systems, where the first SGU is used to generated the HD decoupling and the second to generate the cpd sequence, but the gating of the sequence is taken from the HD pattern from the first SGU.

2.2.3 Phase Setting in CPD Programs: <u>#addphase</u>, <u>#setphase (AV I and AV II only)</u>

The phase specified within a CPD program can be added to the phase

```
1 pcpd*2:sp15:0          1 pcpd*14.156:sp15:60
  pcpd*2:sp15:0            pcpd*14.156:sp15:150
  pcpd*2:sp15:180          pcpd*14.156:sp15:0
  pcpd*2:sp15:180          pcpd*14.156:sp15:150
  pcpd*2:sp15:180          pcpd*14.156:sp15:60
  pcpd*2:sp15:0          2 pcpd*14.156:sp15:240
  pcpd*2:sp15:0            pcpd*14.156:sp15:330
  pcpd*2:sp15:180          pcpd*14.156:sp15:180
  pcpd*2:sp15:180          pcpd*14.156:sp15:330
  pcpd*2:sp15:180          pcpd*14.156:sp15:240
  pcpd*2:sp15:0            lo to 2 times 2
  pcpd*2:sp15:0          3 pcpd*14.156:sp15:60
  pcpd*2:sp15:0            pcpd*14.156:sp15:150
  pcpd*2:sp15:180          pcpd*14.156:sp15:0
  pcpd*2:sp15:180          pcpd*14.156:sp15:150
  pcpd*2:sp15:0            pcpd*14.156:sp15:60
jump to 1                jump to 1
```

Table 2.5 MLEVSP and MPF7 CPD sequences

specified in the pulse program (#addphase) or it can overwrite the pulse program phase (#setphase). Note that #addphase is the default mode. It only needs to be specified if #setphase was used and you want to switch back to #addphase.

Example 1:

Pulse program statement to start the CPD sequence:

d1 cpds2:f2 ph2

CPD program statements:

#addphase
pcpd:180

Resulting phase of the pcpd pulse: 180 plus the current phase in ph2.

Example 2:

Pulse program statement to start the CPD sequence:

d1 cpd2:f2 ph2

CPD program statements:

```
#addphase
pcpd:sp15
```

Resulting phase of the pcpd shaped pulse: shaped pulse phase (according to the phases in the shape file) the current phase in plus ph2.

Example 3:

Pulse program statement to start the CPD sequence:

```
d1 cpd2:f2
```

CPD program statements:

```
#setphase
pcpd:sp15:180
```

Resulting phase of the pcpd shaped pulse: shaped pulse phase (according to the phases in the shape file) plus 180.

Please note that, on Avance-AQX, a phase program should not be used with a cpd*n* statement since the FCU does not support the real-time addition of more than two phases. On Avance-AQS, however, you can use cpd*n* statements with phase programs.

2.2.4 Frequency Setting in CPD Programs

There are three ways to change the frequency of the channel where the CPD sequence is applied. Frequency setting in CPD programs is the same as in pulse programs except that the channel specification after the statement is not necessary.

2.2.4.1 Frequency Setting from Lists

The first method to set the frequency is using a frequency list. The statements fq1-fq8 interpret the parameters FQ1LIST-FQ8LIST, set the frequency from the current list entry and move the list pointer to the next entry. In contrast to the lists used pulse programs, lists used in CPD programs are expanded at compile time, not at run time. In the following example, the

first fq1 statement uses the first entry of the frequency list, the next statement the second entry. If the frequency list contains more than 2 entries, only the first two will be used.

```
1 pcpd:0 fq=fq1
  pcpd:180 fq=fq1
  jump to 1
```

Like in pulse programs, the frequency offset can be specified in two ways: either the offset is at the top of the list in MHz, or no offset is specified in the list. In the latter case, the measure frequency of the appropriate channel (SFO1 for F1, SFO2 for F2, etc.) is used as list offset.

2.2.4.2 Frequency Setting Using the Parameters CNST0-63

The statement fq=cnst25 will set the frequency SFO1 + CNST25 [Hz]. The parameter CNST25 can also be modified from the *gs* window. If used on channel F2, the basic frequency SFO2 instead of SFO1 will be used etc.

2.2.4.3 Direct Specification of Frequencies

The statement fq=3000 will set the frequency SFO1(2,3...) + 3000 Hz.

2.2.5 Loop Statements in CPD Programs

The general form of a loop statement is:

lo to *label* times *n*

where *label* can be any number. The loopcounter *n* can be a number or a symbolic loopcounter l0 - l31, where the latter interpret the parameters L[0] - L[31]. It must be equal to or greater than 1.

Loop counters defined in the pulse program can also be used in the CPD program.

For infinite CPD programs (which are terminated from the pulse program by the statement do:fn) there is a special jump to label statement which executes an unconditional jump to the specified label. For calculated jumps forward (see next section), there exists the command jumpf ln where ln is a loopcounter L0 .. L31.

2.2.5.1 Manipulation of Loop Counters During Execution (BILEV Decoupling)

You can manipulate the loopcounter of a CPD program after each scan according to an arithmetic expression in the following way (this statement must be on the first line of the CPD program):

```
bilev: "l5=nsdone%4+1"
```

This means that the loopcounter l5 will be modified after each scan according to the above equation. The modification will take effect immediately after the scan. The expression should be written such that the loopcounter is always greater than zero. The variable loop counter then can be used within the CPD program such that the first section changes with each scan. This can be done in two ways:

- the CPD program contains a loop using this loop counter.
- the CPD program uses a jump instruction to jump to a calculated label:

```
bilev: "l31=nsdone%4+1"
jumpf l31
1 pcpd*3:180
  pcpd*4:0
...
2 pcpd*2:0
...
3 pcpd*3:180
...
```

The jumpf l31 instruction has the effect that the cpd program continues at the label which corresponds to the current value of the loopcounter calculated above. Of course, each possible loopcounter value must have a corresponding label.

A bilev statement in a CPD program automatically changes the cpd statement in the pulse program into the corresponding cpds. This means that the CPD sequence is not continued at the point where it was stopped before, but starts from the beginning each time it is called.

Chapter 3

Loops and conditions

3.1 Loop statements

The general form of a loop statement is:

    lo to label times n

Example 1:

    label1, d1
         p1:f2
         lo to label1 times 10
         p2:f2

Note that a label can be an arbitrary string, such as label1, followed by a comma, or a number, such as 2, without a comma. The lo statement in this example, although specified on a separate line, does not cause an extra delay between the p1 and p2 pulse statements.

Example 2:

    label1, p1:f1
    label2, d1
         p1:f2
         lo to label2 times 10
         lo to label1 times 5

p2:f2

The first lo statement in this example does not cause an extra delay in the pulse program. However, any further lo statement will add a delay of 2.5 msec. XWIN-NMR will display a corresponding message when the pulse program compiler is invoked, i.e. when entering one of the commands **gs**, **zg**, **go**, or **pulsdisp**.

The lo statement exists in a number of variations as shown in Table 3.1.

`lo to label times 5`	The loop counter is a constant.
`lo to label times td`	The loop counter is TD, the time domain size in the acquisition dimension (to be set with the command **td**, or in the left column in **eda**).
`lo to label times td1`	Only used in 2D or 3D pulse programs. The loop counter is F1-TD (to be set with command **1 td** for 2D data sets or in the right column in **eda**).
`lo to label times nbl`	The loop counter is the parameter NBL (see the statements `wr`, `st`, `st0`)

`lo to label times l0`
 `...........`
 `lo to label times l31`
	The loop counter is L[0] - L[31] (to be set with the commands **l0**, ..., **l31**, or the L array in **eda**). The pulse program statements `iu0`- `iu31` increment the counters `l0`-`l31` by 1, `du0`-`du31` decrement them by 1, and `ru0`-`ru31` reset them to L[0] - L[31].

`lo to label times c`	The loop counter is taken from the list defined by the acquisition parameter VCLIST. The list can be created with **edlist vc**. The statement `ivc` advances the list pointer by 1. The list pointer position can also be set with an equation, e.g. `vcidx=5`.

`lo to label times myCounter`	The loop counter must be defined at the beginning of the pulse program by means of a `define` statement and an expression, e.g.
	 `define loopcounter myCounter`
	 `"myCounter=aq/10m +1"`
	 The result of the expression must be dimensionless.

Table 3.1 The lo statements

Example 3:

```
        ze
label1, (d1 p1):f1
        lo to label1 times l2
        1u iu2
        p2:f2
        go=label1
```

Assume the parameter L[2] is set to 1 using the command *l2 1*, or by setting L[2]=1 in *eda*. Then, (d1 p1):f1 would be executed once before scan 1, twice before scan 2 etc. The lo statement does not cause an extra delay in the sequence. The increment statement iu2 is executed during the specified 1 msecond delay. You could replace the loop counter l2 with c in this example, and replace iu2 with ivc to use the number of loops specified in a list file.

Example 4:

```
define loopcounter myCounter
"myCounter=aq/10m +1"
        ze
label1, (d1 p1):f1
        lo to label1 times myCounter
        go=label1
```

Here the variable *myCounter* represents a loop counter. An arithmetic expression assigns a value to it: the parameter AQ, divided by 10 millisec, plus 1. The compiler truncates the quotient aq/10m to give an integer. The expression may include any of the parameters shown in Table 1.3.

3.2 Conditional pulse program execution

3.2.1 Conditions evaluated at precompile time

Consider the pulse program at the left part of Table 3.2. It combines two experiments in one pulse program, a simple Cosy and a Cosy with presaturation during relaxation. The required pulse program statements to select or deselect presaturation are:

```
#define PRESAT            #define PRESAT

1 ze                      1 ze
2 d11                     2 d11
3 0.1u                    3 0.1u
#ifdef PRESAT             #include <Presat.incl>
  d12 pl9:f1                p1 ph1
  d1 cw:f1                  d0
  d13 do:f1                 p0 ph2
  d12 pl1:f1                go=2 ph31
#endif                     d11 wr #0 if #0 id0 zd
  p1 ph1                   lo to 3 times td1
  d0                     exit
  p0 ph2
  go=2 ph31
  d11 wr #0 if #0 id0 zd
  lo to 3 times td1
exit
```

Table 3.2 Using `#define`, `#ifdef`, `#include` statements

```
#define aFlag
#ifdef aFlag
#ifndef aFlag
#endif
```

and correspond to C language pre-processor syntax where it is mandatory that the "#" is the very first character on the line. Note that *aFlag* is just a place holder, it can be any name. If the pulse program contains the statement:

```
#define aFlag
```

the identifier *aFlag* is considered to be *defined*, otherwise it is considered to be *undefined*. If *aFlag* is *undefined,* the statement:

```
#ifdef aFlag
```

causes the pulse program to ignore all subsequent statements until the statement:

```
#endif
```

If *aFlag* is *defined,* these statements will be executed. The statement:

        #ifndef aFlag

has the opposite effect.

In Table 3.2, #define PRESAT enables the presaturation statement block. Commenting out this line in C-syntax style (/*#define PRESAT*/), (not in pulse program style ;#define PRESAT), would make the PRESAT flag undefined, and the presaturation block would not be executed.

The #ifdef and #ifndef statements are evaluated by a pre-processor. The pulse program compiler will use the pre-processed pulse program. For this reason, these statements do not cause any timing changes. You can view a pre-processed pulse program from the pulse program display. Just enter the **pulsdisp** command and and click the button **Show program**. Note that in the pre-processed pulse program, all conditional statements beginning with a '#' have been removed.

The example could be extended to include double quantum filtering. For this purpose, an additional flag (e.g. #define DQF) could be defined.

The right part of Table 3.2 shows the same pulse program in a more condensed form. The presaturation block is now contained in a separate file, *Presat.incl*, which is included with the #include statement.

3.2.1.1 Setting of Precompiler Conditions

Conditions can be set or unset not only within the pulse program but also on the command line with the **zg** command using the option **-D**. For example, the command **zg -DDQF** has the same effect as the line:

        #define DQF

at the beginning of the pulse program. The argument must follow the **-D** option with or without white space in between. The -D option can be given more than once. As an alternative to command line options to **zg**, you can also set the acquisition parameter ZGOPTNS. Once this parameter is set, the corresponding option is used by **zg** and **go**. Thus, setting ZGOPTNS to "-DDQF -DPRESAT" and typing **zg** has the same effect as the command '**zg -DDQF -DPRESAT**'.

Please note:
All statements beginning with a '#' character must start at the beginning of

a line. Spaces or tabs before '#' are not allowed.

3.2.1.2 Macro Definitions

You can use the statement #define not only to define *a flag*, but also, as in C language, to define a macro.

Example 1:

```
#define macro1 (p1 d1) (p2):f2
macro1
```

This pulse program section is equivalent to:

```
(p1 d1) (p2):f2
```

Example 2:

```
#define macro2 (p1 d1) \n\
        (p2):f2
macro2
```

This pulse program section is equivalent to:

```
(p1 d1)
(p2):f2
```

The definition of macro2 extends over 2 lines using the \n\ character sequence. In example 1, p1 and p2 start at the same time, while in this example p2 starts after (p1 d1) has finished.

Example 3:

```
#define macro3 (p1 d1) \n (p2):f2
macro3
```

This pulse program is equivalent to:

```
(p1 d1)
(p2):f2
```

The definition of macro3 requires only one line. However, the \n character sequence enforces a new line when the macro is evaluated. As such, the pulse programs of the examples 2 and 3 are identical.

Attention: Macro symbols are replaced by the body of the macro everywhere in the text, even in comments and strings. If you use a macro in a comment, where you don't want it to be replaced, you should use a C-style

comment instead.

Example:

    ; the macro3 produces two pulses on two channels

This will be expanded by the precompiler to

    ; the (p1 d1)
    (p2):f2 produces two pulses on two channels

which will produce a syntax error. The following statement is correct:

    /* the macro3 produces two pulses on two channels */

because the C-precompiler removes the line entirely.

3.2.2 Conditions evaluated at compile time

Whereas conditions controlled by #if statements are evaluated at precompile time, conditions controlled by if statements are evaluated at compile time.

The if statement can be used in connection with the parameters L[0] - L[31] as shown in the following example:

`if (l7==0)`	if l7 is zero
`if (l8!=0)`	if l8 is not zero
`if (l9 op(`*arith. expression*`))`	`op` can be ==, !=, >, <, >=, or <=

Table 3.3

The condition must be followed by an if-block and, optionally, can be followed by an else-block. The statement 'else if', as it is used in C language, is not allowed in pulse programs.

Example: See Table 3.4

The if-block is executed if the condition is true at compile time; in the above

```
if (l5 > 2)
{
  p1 ph1
}
else
{
  p1 ph2
}
```

Table 3.4 a condition evaluated at compile time

example if l5 is greater than 2, p1 is executed with phase program ph1, if not, it is with phase program ph2. If l5 changes during the experiment, and the condition becomes false, the execution mode doesn't change.

3.2.3 Conditions evaluated at run time

The spectrometer TCU has four trigger inputs. Trigger events can be positive or negative edges or levels.

XWIN-NMR supports branching and evaluation of conditions within a pulse program while the pulse program execution is in progress. Table 3.5 lists the available statements. These statements do not cause a delay in the pulse program. At run time, pre-evaluation is performed during the cycle time of the loops in which the statements are embedded. If, in a particular pulse program, loops are executed too fast, a run time message is printed.

Example 1:

```
      ze
lab1, d1
      p1
      d0
      if "d0*2 + 7m > 500m" goto lab2
      "d0 = d0 + 10m"
      p2
lab2, go=lab1
```

Assume that we will start with d0=10m. The pulse p2 will no longer be executed when the expression "d0*2 + 7m > 500m" becomes true.

Example 2:

`goto label`	Unconditional jump to `label`
`if expression goto label`	Branch to `label` if `expression` evaluates to *true*.

`if (trigger) goto label`	Branch to `label` if the `trigger` condition is true.
	Positive *level trigger* specifiers:
	`trigpl1, trigpl2, trigpl3, trigpl4`
	Negative *level trigger* specifiers:
	`trignl1, trignl2, trignl3, trignl4`

`aDelay trigger`	The same `trigger` specifiers as above are allowed. The next pulse program statement will not be executed until the `trigger` condition becomes *true*. Example:`1u trigpl1`
	Positive *edge trigger* specifiers:
	`trigpe1, trigpe2, trigpe3, trigpe4`
	
	Negative *edge trigger* specifiers:
	`trigne1, trigne2, trigne3, trigne4`

Table 3.5 Conditional pulse program execution

```
      ze
lab1, if (trigpl2) goto lab3
lab2, d1
      p1
      aq
      lo to lab2 times ds
      goto lab1
lab3, d1
      p1
      go=lab1
```

The TCU has 4 trigger input channels (on the TCU3 they are numbered 0-3 and correspond to the trigger commands 1-4); signals arriving at the TCU can be checked using the trig specifiers. This example performs DS dummy scans to maintain steady state conditions as long as no positive level is detected on input channel 2. If such a level is detected, NS data acquisition scans are executed,

then the pulse program again checks the external trigger signal.

Example 3:

```
      ze
lab1, d1 trigpl2
      p1
      go=lab1
```

This example starts executing the pulse sequence as soon as a positive level is detected on input channel 2. After each scan, the pulse program will wait until the next trigger signal is detected.

Example 4:

```
      ze
lab1, d1
      p1
      lo to lab1 times l2
      0.1u iu1                          ;count number of scans
      0.1u iu2                          ;increment l2
      if "l1 <= 3" goto lab2            ;if scancounter < 4
      0.1u ru2                          ;reset l2 to L2
lab2, go=lab1
```

This example repeats the sequence (d1 p1) L[2] times before scan 1, L2+1 times before scan 2, and L2+2 times before scan 3. Then, l2 is reset to its initial value L[2]. Before all remaining scans the sequence (d1 p1) is generated L[2] times. L[1] must be set to 1 before starting the sequence.

3.3 Suspend/resume pulse program execution

XWIN-NMR allows you to stop (suspend) the pulse program execution at specified positions in the pulse program. Pulse program suspension can be done conditionally or unconditionally using the statements shown in Table 3.6.

After suspension, the program execution can be resumed with the XWIN-NMR command *resume*.

If you use suspend or autosuspend, you should not try to change any acqui-

suspend	stop execution on the command ***suspend***
autosuspend	stop execution
calcsuspend	stop precalculation and stop execution on ***suspend***
calcautosuspend	stop precalculation and stop execution

Table 3.6 statements to suspend pulse program execution

sition parameters between suspending and resuming the acquisition, because this will not have the wanted effect. The reason is that the acquisition uses the principle of precalculation which means a part of the pulse program is interpreted (precalculated) before it is actually executed. After resume, the precalculated part which was calculated before the parameter change is executed without considering the parameter change.

The statement calcsuspend or calcautosuspend, however, stop precalculation. Here you can change parameters between suspending and resuming the acquisition. Note that you must specify a delay which is long enough to start and do a reasonable amount of precalculation after ***resume***. For example:

```
calcsuspend
2s
```

If, after resuming the acquisition, you would get the error message "timing too short", you must increase this delay.

Chapter 4

Data acquisition and storage

4.1 Start data acquisition

XWIN-NMR provides 5 basic pulse program statements to start data acquisition:

go=*label*, gonp=*label*, gosc, goscnp and adc.

The most commonly used statement is go=*label*. Actually, go is a macro statement, i.e. it includes a number of different actions required for data acquisition. The statement adc can be used to control fine details of the acquisition process. All five acquisition statements place the digitized signal into a memory buffer. The wr statement, described in a later section, writes the buffer contents to disk.

4.1.1 The statements **go=*label*, gonp=*label*, gosc, goscnp**

The left column of Table 4.4 shows a simple example of how to use go=*label* in a pulse program. All go type statements perform the 8 actions described below. A parallel sequence of 5 pre-scan subdelays is executed (see the description of DE1/DERX/DEPA/DEADC in the Acquisition Reference Manual). Note that all these delays end simultaneously, at the end of DE. The sequence in which the actions are performed, depends upon the length of

the individual delays. The sequence must be

$$DE > DEPA \geq DE1 \geq DERX \geq DEADC$$

1. At the end of DE-DEPA (preamplifier blanking delay), the preamplifier is switched to observe mode.

2. At the end of DE-DERX (delay for receiver blanking) the receiver gate is opened.

3. At the end of DE-DE1, the intermediate frequency (if used) is added to the frequency of the observe channel and the observe SGU switches from transmit to observe mode. This corresponds to the execution of the statement syrec. The intermediate frequency is only used for AQ_mod = DQD.

4. At the end of DE-DEADC (delay for ADC blanking), the digitizer is enabled.

5. After a total delay of DE the digitizer is started. Please refer to the description of the parameters DW/DWOV/DIGMOD on how the sampling rate is selected. The result will be a digitized FID signal of TD data points, where the time domain size TD is defined by the user (from **eda**, or by typing **td**). The FID will be put into the *current memory buffer*. The contents of memory buffers can be transferred to disk with the wr pulse program statement or with the **tr** command. The section *Acquisition memory buffers* discusses the usage of memory buffers and the size restrictions of TD.

6. At the time the digitizer is started, a delay AQ is executed. This delay lasts until the digitization of the FID is finished.

7. A delay of 3 millisec is executed. During this time the following tasks are performed:

   a) The scan counter, visible during real time FID display, is incremented to inform the user about the number of scans performed since the last executed ze or zd statement.

   b) The frequency of the observe channel is switched back to the frequency of the observe nucleus (if the intermediate frequency is used). This corresponds to the execution of the statement sytra (which is inverse to syrec). The intermediate frequency is only used for AQ_mod = DQD or, if your spectrometers has an RX22 receiver, for any value of AQ_mod.

c) The pointers of all phase programs are incremented to the next phase, corresponding to the execution of the statements ipp0, ... , ipp31. This step is skipped by gonp=*label* and goscnp.

d) The statements go=*label* and gonp=*label* perform a loop to *label*, whereas gosc and goscnp do not loop. The pulse program statements between *label* and go or gonp are executed DS+NS times. During the first DS loops (*dummy scans* to achieve steady state conditions), the digitizer is not activated. In all other respects, the dummy scans are identical to the NS data acquisition scans. If no dummy scans are desired, DS must be set to 0.
Please note: Even if DS > 0, no dummy scans will be executed if the pulse program statement zd (rather than ze) was executed before a go loop is entered (see the description of ze and zd). This feature is, for example, used in 2D experiments where dummy scans are only required before the first FID is measured.

e) Commands after an additional finally statement are executed during this delay. In this way decoupling can be switched on during the acquisition time only and need not be terminated outside the go command.

Table 4.1 shows that the go statements can be specified in conjunction with other statements. PH_ref is an acquisition parameter to be defined by the user.

4.1.2 The statements rcyc=*label*, rcycnp=*label*

The statement rcyc executes step 7 of the actions performed by go=*label* and gonp=*label* (see the previous section). The rcycnp statement skips step 7c.

The rcyc statements can be used for acquisition loops based on adc rather than go=*label* or gonp=*label*. You must *not* specify phase programs behind rcyc and rcycnp. Decoupling statements are allowed although it would not make sense to use them here. Table 4.4 shows an example of an acquisition loop with rcyc. Note that the adc statement is part of the DE1 macro statement.

The rcyc statements can also be specified behind a delay, e.g. 100u rcyc=2. They are then executed during that delay instead of the default 3 millisec.

1	`go=2 ph31`	Receiver phase = ph31, realized via add/ subtract and channel A/B switching. Allowed phase values: 0, 90 180, 270 degrees.
2	`go=2 ph30:r`	Receiver phase = ph30 + PH_ref, realized via the phase of the reference frequency of the observe channel. Allowed phase values: any.
3	`go=2 ph31 ph30:r`	Combination of (1) and (2). The receiver phase is the sum: ph31 + ph30 + PH_ref
4	`go=2 ph31 ph30:r cpd1:f2`	Decoupling starts at the same time the receiver is opened, and automatically stops when the loop is executed.
5	`go=2 ph31 ph30:r cpd1:f2 ph29`	As example 4, with a phase program for the CPD sequence.
6	`go=2 cpd1:f2 finally do:f2`	As example 4, but decoupling ends after the acquisition time

Table 4.1 Examples of the usage of the `go` or `gonp` statement

Such a delay must be at least 100 msec.

4.1.3 The statements <u>eosc,</u> <u>eoscnp</u>

The statement eosc executes steps 7a-7c of the actions performed by go=*label* and gonp=*label* (see the previous section). The eoscnp statement only executes steps 7a and 7b.

The eosc statements can be used in pulse programs with data acquisition based on adc. In contrast to rcyc, you must add the appropriate loop statements.

You must *not* specify phase programs behind eosc and eoscnp. Decoupling statements are allowed but it would not make much sense to use them here. Table 4.4 shows an example of an acquisition loop based on eosc. Note that the adc statement is part of the DE1 macro statement.

The statement eosc or eoscnp can also be specified behind a delay of at

least 100 msec, e.g.:

        100u eosc

In that case, they are then executed during the specified delay rather than during the default 3 millisec.

4.1.4 The statements `ze` and `zd`

The statements ze and zd perform the following actions:

1. They set the scan counter, which is visible during real time FID display, to 0 or to -DS. A negative value indicates that dummy scans are in progress.

2. They set a flag which triggers the next go, gonp, gosc, goscnp, or adc statement to <u>replace</u> any existing data in the acquisition memory rather than add to them. This counts for all NBL memory buffers. If ze or zd are placed outside an acquisition loop, the *replace* mode will only be valid for the first scan performed by the loop. The FID's of all the scans that follow will be added to the data present in the memory buffer.

3. The statement zd automatically resets all phase program pointers to the first element, whereas the statement ze sets all phase program pointers such that they are at the first element after DS dummy scans.

4. The difference between ze and zd is that zd prevents the execution of dummy scans by go, gonp, gosc, goscnp, and by adc (combined with rcyc or eosc), even if DS > 0.

The statements ze and zd can be written behind a delay statement. They are then executed during the delay. If they are not specified with a delay their execution will require 3 millisec.

The statement zd is normally part of one of the specifications of the mc macro statement. One example where it is specified explicitly is the pulse program *selno*.

4.1.5 The statement <u>adc</u>

The statement adc starts the digitizer and, at the same time, opens the receiver. Please refer to the description of the parameters DW/DWOV/DIG-MOD in the Acquisition Reference Manual for information on how the sam-

pling rate is calculated. The result of adc will be a digitized FID signal of TD data points. TD is an acquisition parameter that must be set by the user. The FID will be placed in the current memory buffer (see the section *Acquisition memory buffers*).

When you use the adc statement rather than go, you must consider the following:

- Whereas the go statement automatically executes the required switching delays, these must be specified explicitly when you use adc. For this purpose, the macros DE1, DE2, DE3, DEPA, DERX and DEAC are available. They are defined in the file *De.incl* that can be included in the pulse program with the statement:

  #include <De.incl>

  The contents of this file is shown in Table 4.2.

```
define delay rde1
define delay rdepa
define delay rderx
define delay rdeadc

"rde1=de-de1;"
"rdepa=de-depa;"
"rderx=de-derx;"
"rdeadc=de-deadc;"

#define DE1(phrec) (rde1 de1 adc phrec syrec)
#define DE2(phref) (1u 1u phref:r):f1
#define DE3 (de)
#define DEPA (rdepa depa RGP_PA_ON)
#define DERX (rderx derx RGP_RX_ON)
#define DEADC (rdeadc deadc RGP_ADC_ON)

#define ACQ_START(phref,phrec) DE1(phrec) DE2(phref) DERX
DEADC DEPA DE3
```

Table 4.2 The contents of the file De.incl for AV and AV-II spectrometers

*Note that **adc** is implicitly defined with **DE1***

Here, the statement de executes the delay defined by the acquisition parameter DE. The statements de1, derx, deadc and depa execute a delay that is defined by the corresponding *edscon* parameters. In the

```
define delay rde1

"rde1=de-de1"

#define DE1(phrec)    (rde1 sync de1 adc phrec syrec)
#define DE2(phref)    (1u 1u phref:r):f1
#define DE3    (de)

#define ACQ_START(phref,phrec) DE1(phrec) DE2(phref) DE3
```

Table 4.3 The contents of De.incl for AV-III spectrometers

case of an AV-III spectrometer, the three delays DEPA, DERX and DEADC are generated automatically by the hardware and can be replaced by one single DE2. The DE1 and DE2 macros have the arguments phrec and phref which are used to define the phase program used by the receiver and the reference frequency, respectively. The latter phase program can be specified after the go macro using the syntax ph*nn*:r.

- For end-of-scan handling, you must specify one of the statements eosc, eoscnp, rcyc, or rcycnp. Multiple adc statements can be used in conjunction with, for example, a single eosc statement. Table 4.4 shows the same pulse program realized via go=*label*, adc in conjunction with rcyc, and adc in conjunction with eosc.

- You must enable the intermediate frequency using the statement syrec. This, however, is only necessary for AQ_mod = DQD or, if your spectrometers has an RX22 receiver, for any value of AQ_mod.

- The dwell time is generated during aq. For Avance-AQX, the adc statement starts dwell generation on the RCU (here the macro DWELL_GEN has no effect). For Avance-AQS, the dwell time is generated on the SGU with the macro DWELL_GEN.

| ```
   ze
2 d1
   (p1 ph1):f1
;---------
   go=2 ph31
;--------
   wr #0
   exit
``` | ```
#include De.incl
 ze
2 d1
   (p1 ph1):f1
;------------------
 DE1 DEPA DERX DEADC DE3
  aq DWELL_GEN
  rcyc=2
;------------------
   wr #0
   exit
``` | ```
#include De.incl
   ze
2 d1
   (p1 ph1):f1
;------------------
DE1 DEPA DERX DEADC DE3
  aq DWELL_GEN
  eosc
  lo to 2 times ns
;------------------
   wr #0
   exit
``` |

Table 4.4 The same pulse program based on `go`, `adc/rcyc`, and `adc/eosc`

For an example of how to use the `adc` statement rather than `go`, please look at the Bruker pulse program *zgadc* (enter **edpul zgadc**). This program will produce exactly the same result as the program *zg*.

4.1.5.1 The receiver phase

In pulse programs using the `adc` statement, the receiver phase must be specified behind `adc`, e.g.:

   adc ph31

This statement tells the receiver which phase is to be used for the next scan to account for the receiver phase setting. Note that there must be sufficient time between the end-of-scan interrupt signal of one scan and the receiver phase interrupt signal of the next scan. Normally, the recycle delay is long enough for this purpose. However, for some applications (like imaging experiments) the recycle delay can be too short for correct interrupt handling. In that case, the receiver phase should be specified before the scan loop using the statement recph ph31 (see Table 4.5). The statement ip31 after the recycle loop increments all entries of the phase program ph31 but does not set the phase. As such, the receiver phase is not changed after each scan but after NS scans.

4.1.6 Real Time Control

On spectrometers equipped with a DRU-M unit and an Real-Time-Control-

```
1 ...                      1 ...
  ...                        ...
2 d1                         2u recph ph31
  10u adc ph31             2 d1
  aq DWELL_GEN:f1            10u adc
  rcyc=2                     aq DWELL_GEN:f1
  10u ip31                   d2 rcyc=2
  lo to 1 times l1           10u ip31
  ...                        lo to 1 times l1
                             ...
```

Table 4.5 Receiver phase setting without and with `recph`

ler board (RCTRL), the command *rcen*, issued before an acquisition command (*adc/go*), will cause the next scan to be transferred from the addressed DRU-unit to the connected RCTRL board. There are no specific timing requirements for the command.

Example:

    1u rcen   ; transfer scan to R-Controller
    go=1

4.1.7 External dwell pulses

The `go` and `adc` statements instruct the digitizer to acquire the desired number of data points with a rate given by the *dwell time*. On AQX systems, the dwell pulses, which activate the digitizer in regular time intervals, are generated internally (on the RCU) so that the detection of a complete FID is automatically accomplished once initialized via `go` or `adc`. This occurs during the delay `aq` as displayed in the middle and the right columns of Table 4.4. On AQS systems, the dwell pulses are generated by the SGU which is dedicated to the observe channel. This is the meaning of the macro DWELL_GEN which evaluates to the statement:

    aq cpdngs29:f1

Certain experiments, however, require the control of the detection of each

individual data point of an FID. In this pulse program the waiting time aq has been replaced by a loop that generates as many dwell pulses as required to measure TD data points. Use the command setrtp to generated the dwell pulses and the receiver gating pulses.

Please refer to the Bruker pulse program libraries for high resolution, solids, and imaging experiments for examples using the the setrtp command.

For AV II and AV III systems, the digitizer has a constant rate of 20 MHz and cannot be stopped and started, instead it can be gated and the resulting data stream is filtered and decimated according to the chosen sweep width and decimation. If single data points are needed, for each gating pulse ANAVPT points of the digitizer can be averaged to one resulting point. Therefore for DRU systems, if DIGMOD is set to analog, there must be a statement like

        "anavpt=512"

in the pulse program which tells the digitizer how many points should be averaged. The generation of the dwell pulses can be done as described above.

4.2 Acquisition memory buffers

The acquisition statements go=*label*, gonp=*label*, and adc put the acquired data points into a *memory buffer* where they reside until new data points are added, or until they are replaced by new data (*replace* mode is turned on by the statements ze and zd). A memory buffer provides space for TD data points, where TD must be set by the user.

In most 1D experiments, one FID is measured and stored in one memory buffer. After NS scan have been accumulated, the contents of that memory is written to disk (with the wr statement). Multi-dimensional experiments, imaging experiments, experiments varying parameters such as the decoupling frequency or recovery time generate several FID's. In that case you can use one or several memory buffers. If a single buffer is used, the buffer contents must be transferred to disk before the next FID can be measured. If several buffers are used, several FID's can be measured before a disk transfer is required. The latter method is appropriate if the FID's of the experiment succeed one another so quickly that no disk transfer is possible

in between them.

The acquisition parameter NBL determines the number of memory buffers used (default: NBL=1). Each buffer has a size TD. If TD is not a multiple of 256, the buffer size will be rounded to the next multiple of 256 data points . The acquisition commands will put the FID into the *current* buffer. The default *current* buffer is buffer 1. The pulse program statement st makes the *next* buffer the current buffer whereas the statement st0 makes the *first* buffer the current buffer. When the number of buffers is exhausted, i.e. when st is executed for the NBL'th time, the *first* buffer becomes the current buffer.

The statements st and st0 must be specified behind a delay which must be at least 10 msec, e.g.:

    10u st

Table 4.6 shows an example, the Bruker pulse program *noedif*. The FID's

```
1 ze
  d11 pl14:f2
  d11 fq2:f2 st0
2 d1
3 d20 cw:f2
  d13 do:f2
  p1 ph1
  go=2 ph31
  d1 fq2:f2 st
  lo to 3 times l4
  d11 wr #0 if #0
exit
```

Table 4.6 Usage of st and st0: *noedif* pulse program

acquired with different decoupling frequencies are stored in two memory buffers.

The size of NBL is limited by the constraint that NBL times TD must not exceed the available RCU or DRU memory. For example, an RCU equipped with 4 Mb DRAM allows for about 3.8 Mb FID data to be stored

(the remainder is needed by the acquisition parameters). If necessary, you can upgrade your spectrometer with more RCU DRAM.

The commands ze and zd reset the scan counters for all nbl buffers. Of course, the pulse program must do ns (ns+ds) scans in each buffer before advancing to the next buffer with the command st. If dummy scans should be done only before acquisition starts in the first block, it is better to write a separate loop before the actual acquisition loop in the pulse program.

4.3 Writing data to disk

Data acquisition statements go=*label*, gonp=*label*, gosc, goscnp, and adc put the digitized data into a memory buffer, but do not store them to disk. Therefore, every pulse program must contain at least one disk write statement to transfer the acquired data to disk. Table 4.7 shows the available pulse program statements to access disk files.

Transferring data to disk means *adding* the data to the data contained in an existing *fid* or *ser* file, or *replacing* these data.If no such file exists, it will be created. *Replacement* will take place if started with **zg**, *addition* will take place if the pulse program is started with the command **go**. However, data replacement only occurs the first time a memory buffer is transferred to disk. Any further execution of the mc or wr statement will cause the buffered data to be added to the data in the file.

It is allowed to specify the statements if, zd, id0-id31, ip0-ip31, and decoupling statements behind the same delay that is used for wr. It is important to use either a zd or ze statement after each wr before the next scan. Otherwise the data will be added to data previously acquired in the same memory region.

The name of the output file is *fid* or *ser*. An *fid* file contains a single FID, whereas a *ser* file contains a series of FID's. The appropriate name is automatically chosen by the pulse program compiler: if a pulse program contains one of the increment, decrement, or reset file pointer statements, or st/st0, a *ser* file will be created.

If the pulse program uses a *ser* file, the acquisition command checks if a ser file already exists and if it has the correct size. If this is the case, the

`mc #0`	Macro statement that executes the statements `wr #0`, `if` and `zd`. Normally `mc` is specified with one or more clauses which expand to loop structures.
`wr #0`	Transfer the acquisition buffer to the file *fid,* or transfer NBL acquisition buffers to the file *ser* of the *current* data set. For *ser* files: `wr` starts writing into the file at the current position of the *disk file pointer*, which initially is at the beginning of the file.
`wr #1, wr #2, wr #3, ...`	Transfer is performed to the file *fid* or *ser* of the data set with the number 1, 2, 3, ... contained in the data set list defined by the acquisition parameter DSLIST.
`wr ##`	Transfer is performed to the file *fid* or *ser* of the data set which is pointed to by the *dataset list pointer*. Its initial position is #0 which always corresponds to the foreground dataset. The dataset list pointer itself can be manipulated with the commands `ifp`, `rfp` and `dfp`.
`if #0, if #1, if #2, ...`	Advance the *disk file pointer* for *ser* files by TD*NBL (note that TD is rounded to the next multiple of 256 data points if it is not a multiple of 256).
`if ##`	Advance file pointer of current file (see `wr ##`)
`df #0, df #1, df #2, ...`	Decrement the file pointer (inverse of `if`).
`rf #0, rf #1, rf #2, ...`	Reset the file pointer to the beginning of the *ser* file.
`rf #0 m, rf #1 m, rf #2 m, ...`	Set the file pointer to position m*TD*NBL of the *ser* file, where m is an integer number.
`ifp`	The dataset list pointer ## is incremented by 1. It initially points to the foreground dataset (#0), after the first increment to the first item of the dataset list (#1) and so on (NB: there is no automatic wraparound).
`dfp`	The dataset list pointer ## is decremented by 1
`rfp`	The dataset list pointer ## is reset to the first item (the foreground data set #0).

Table 4.7 Writing acquisition buffers to disk

first occurrence of a wr statement will overwrite the *ser* file section defined by the current file pointer, TD, and NBL. If a *ser* file does not exist or has the wrong size, a new *ser* file will be created filled it with zeroes before acquisition starts. As such, the *ser* file is not required to grow during the experiment. This method avoids the risk of running out of disk space while acquisition is in progress.

In a 2D experiment, the TD value must be set such that $TD_{F1}*TD_{F2}*4$ corresponds to the size (in bytes) of the ser file. In a 3D experiment, the TD values must be set such that $TD_{F1}*TD_{F2}*TD_{F3}*4$ corresponds to the size (in bytes) of the ser file. If they are not, a warning is displayed even though the experiment can still be executed. If, for some reason you have performed a 2D experiment with TD values that do not match the size of the ser file, you must set the status TD_{F1} value before you process the data. You can do that with *1s td*. For 3D experiments you can adjust the TD values of the indirect dimension with *2s td* and *1s td*.

These rules apply to acquisition dimensions higher than 3 in a similar way. TOPSPIN allows acquisition dimensions up to 8D.

In 3D pulse programs, the acquisition status parameter AQSEQ describes the order (*321* or *312*) in which the 1D FID's of a 3D acquisition are written into the *ser* file (3 = the acquisition dimension, 1 and 2 = the orthogonal dimensions). AQSEQ is automatically set and stored in the parameter file *acqus* according to the pulse program loop structure. A 3D pulse program usually contains a double nested loop with loop counters td1 and td2. If td1 is used in the inner loop and td2 in the outer loop, AQSEQ is set to 312. Otherwise it is set to 321. Note that in most 3D pulse programs, the td1 and td2 loop is implicitly defined by an mc statement. If a 3D pulse program contains a different loop structure (not defined by td1/t2d or mc) AQSEQ should be explicitly set with one of the statements:

```
aqseq 321
aqseq 312
```

before the actual pulse sequence. Without this statement, the status parameter AQSEQ would be set to an arbitrary value. In that case you can still set it after the acquisition has finished (before processing) is with the command *3s aqseq* . In dimensions higher than 3D only the natural order (e.g. 4321) is supported and there is no corresponding aqsec command.

The wr statements (and all other statements in Table 4.7) can be specified behind a delay (see the example in Table 4.6). The delay must be at least 10 msec. The only timing requirement for wr is that the disk transfer is finished before wr is called again. If it is not, a run-time error message is printed. The actual execution time of a disk write depends on the computer hardware, the operating system, and the system load according to currently active processes and users. Bruker recommends to acquire data only to a disk that is physically connected to the computer that controls the spectrometer.

However, there is another limit if wr is used in conjunction with other commands for data handling. The commands wr, if and zd may be combined on a single line. Other commands, like ze must be on a separate line. Any sequence containing one of these commands more than once must have a delay of 10 ms between two of them.

Chapter 5

The mc macro statement

5.1 The mc macro statement in 2D

A 1D experiment can be based on the following pulse program sequence:

```
1 ze    ; initialisation
2 d1    ; starting delay
  p1    ; pulsing
  d0    ; waiting
  go=1  ; acquiring FID and loop for adding
  d1 wr #0; write to buffer
```

You can turn this sequence into a 2D sequence by taking the following steps:

- increment the file pointer after each disk write
- initialize the buffer after each disk write
- increment a delay, by convention d0, in each loop
- add a loop outside of the wr #0 statement to a second label - the size of which is usually td1
- for phase sensitive acquisition: add a phase increment

When the indirect dimension is acquired phase insensitive, the 2D pulse

program would have the following form:

```
1  ze
2  d1
3  p1
   d0
   go=2
   d1 wr #0 if #0 zd id0
   lo to 3 times td1
```

The last two lines can be replaced by the mc statement. In the above sequence, this would take the form:

```
d1 mc #0 to 2 F1QF(id0)
```

The statement mc is a macro that includes a disk write (wr), a file increment (if) and memory initialization (zd). It can be used with one or more clauses, e.g. F1QF, which expands to a loop structure. Each clause can take one or more pulse program statements, e.g. id0, as arguments. These statements are executed within the loop created by the clause. Different mc clauses are used for phase sensitive, phase insensitive and echo-antiecho experiments. However, the same mc clause, i.e. the same pulse program, can be used for different types of phases sensitive experiments like QSEQ, States, TPPI and States-TPPI. The experiment type is determined by the F1 acquisition parameter FnMODE. The allowed combinations of FnMODE and mc clauses are listed in Table 5.1.

mc clause	Mode	Possible values of FnMODE[F1]
F1QF	phase insensitive	QF
F1PH	phase sensitive	QSEQ, States, TPPI, States-TPPI
F1EA	Echo-Antiecho	Echo-Antiecho

Table 5.1 : allowed combinations of FnMODE and mc clauses

If an incorrect combination of FnMODE and mc clause is used, such as F1PH - QF, the **zg** command will show an error message and quit.

2D and 3D processing commands interpret the acquisition status parameter FnMODE and set the processing status parameter MC2 accordingly. However, if FnMODE = undefined, they interpret the processing parameter

MC2 and set the <u>processing status</u> parameter MC2 accordingly.

By using mc instead of the wr and lo to label statements the same 2D (and 3D) pulse programs can be used for TPPI, States-TPPI and States, respectively. We will look at the expanded forms of cosyph for different values of FnMODE[F1]. The unexpanded pulse program as it appears with ***edpul cosyph***:

```
"d0=3u"

1  ze
2  d1
3  p1 ph1
   d0
   p0 ph2
   go=2 ph31
   d1 mc #0 to 2 F1PH(ip1, id0)
   exit

ph1 =0 2 2 0 1 3 3 1
ph2 =0 2 0 2 1 3 1 3
ph31=0 2 2 0 1 3 3 1
```

The mc command will put into the expanded pulse programs the following header which is the same for the different values of FnMODE[F1]:

```
define delay MCWRK
define delay MCREST
"MCREST = d1 - d1"
```

As such, it is not specified in the expanded pulse programs below. Note that MCWRK, MCREST are general delays that are defined during the expansion of the mc statement. MCREST is zero for all expansions of cosyph but can be non-zero for other pulse programs. MCWRK, however, is different for different expansions. Note that the phase programs are, for each value of FnMODE, the same as in the unexpanded pulse program.

FnMODE[F1] = QSEQ:

```
define loopcounter ST1CNT
"ST1CNT = td1 / ( 2 ) "
"MCWRK = 0.500000 * d1"
        1       ze
```

```
                              "in0 = in0 / 2"
                    2         MCWRK
LBLSTS1,                      MCWRK
       LBLF1,                 MCREST
                    3         p1 ph1
                              d0
                              p0 ph2
                              go=2 ph31
                              MCWRK  wr #0 if #0 zd ip1 id0
                              lo to LBLSTS1 times 2
                              MCWRK rp1
                              lo to LBLF1 times ST1CNT
                              exit
```

FnMODE[F1] = States

```
        define loopcounter ST1CNT
        "ST1CNT = td1 / ( 2 ) "
        "MCWRK  = 0.500000 *  d1"
                    1         ze
                    2         MCWRK
LBLSTS1,                      MCWRK
       LBLF1,                 MCREST
                    3         p1 ph1
                              d0
                              p0 ph2
                              go=2 ph31
                              MCWRK  wr #0 if #0 zd ip1
                              lo to LBLSTS1 times 2
                              MCWRK  rp1 id0
                              lo to LBLF1 times ST1CNT
                              exit
```

FnMODE[F1] = TPPI

```
        "MCWRK  = d1"
                    1         ze
                              "in0 = in0 / 2"
                    2         MCWRK
       LBLF1,                 MCREST
                    3         p1 ph1
                              d0
                              p0 ph2
```

```
                    go=2 ph31
                    MCWRK  wr #0 if #0 zd   ip1 id0
                    lo to LBLF1 times td1
                    exit
```

FnMODE[F1] = States-TPPI

```
        define loopcounter ST1CNT
        "ST1CNT = td1 / ( 2 ) "
        "MCWRK  = 0.500000 * d1"
                1       ze
                2       MCWRK
        LBLSTS1,        MCWRK
           LBLF1,       MCREST
                3       p1 ph1
                        d0
                        p0 ph2
                        go=2 ph31
                        MCWRK  wr #0 if #0 zd ip1
                        lo to LBLSTS1 times 2
                        MCWRK  id0
                        lo to LBLF1 times ST1CNT
                        exit
```

The expanded version of the pulse program can be found in the expno directory of the dataset in the file *pulseprogram*. Note that the mc statement performs the following actions:

- In QSEQ, States, States-TPPI and Echo-Antiecho mode, mc creates two loops and sets the corresponding labels and delays. The delay at the line to which mc loops back to is split into two equal parts: one for the inner loop label and one for the outer loop label.

- For FnMODE[F1] = *QSEQ* or *TPPI*, the value for the delay increment is divided by 2 during run time. The parameter ND0, which represents the number of occurrences d0 within the loop, must have same value for all values of FnMODE.

- For FnMODE[F1] = *QSEQ* or *States*, an rp1 statement is included within the outer loop. This causes the phases of ph1 to be reset to their original values.

- For FnMODE[F1]= *States*, *States-TPPI* and *Echo-Antiecho*, the statements specified in the first argument of the mc clause are exe-

cuted in the inner loop and the statements specified in the second argument are executed in the outer loop.

- For FnMODE = *QSEQ*, the statements specified in the first and second argument of the mc clause are executed in the inner loop.

- For FnMODE = *TPPI*, only one loop is created so the statements specified in the first and second argument of the mc clause are executed in that loop.

- For FnMODE = *QF*, the mc clause contains only one argument whose statements are executed in the only loop that is created.

For large 2D data sets, it is often useful to test the experiment with the first increment. This can be done by setting the parameter TD[F1] to 1. The dimension of the generated dataset will be 1D and can be processed as such. Note that you do not have to change the value of the parameter PAR-MODE; it is still set to 2D. In the same way, you can acquire a plane of a 3D dataset by setting TD[F1] or TD[F2] to 1, and a single row by setting TD[F1] and TD[F2] to 1.

5.2 The mc macro statement in 3D

The mc statement can also be used in 3D pulse programs. In this case, there are two indirect dimensions, F1 and F2. For the F1 dimension, mc uses the clauses F1PH, F1EA and F1QF, for the F2 dimension, it uses the clauses F2PH, F2EA and F2QF.

The F2PH clause creates a second loop within which a second delay is varied.

The pulse program *noesyhmqcpr3d*:

```
aqseq 312

1 d11 ze
2 d11 do:f2
3 d12 pl9:f1 pl2:f2
  ...
    go=2 ph31 cpd2:f2
  d11 do:f2 mc #0 to 2
    F1PH(ip1 & ip29, id0)
```

```
            F2PH(rd0 & ip5, id10)
        exit
```

with

```
   FnMODE[F2] = States-TPPI
   FnMODE[F1] = States-TPPI:
```

expands to:

```
        aqseq 312

        define delay MCWRK
        define delay MCREST
        define loopcounter ST2CNT
        "ST2CNT = td2 / ( 2 ) "
        define loopcounter ST1CNT
        "ST1CNT = td1 / ( 2 ) "
        "MCWRK  = 0.166667 *  d11"
        "MCREST =  d11 -  d11"
                1       d11 ze
                2       MCWRK*2  do:f2
    LBLSTS2,        MCWRK
       LBLF2,       MCWRK*2
    LBLSTS1,        MCWRK
       LBLF1,       MCREST
                3       d12 pl9:f1 pl2:f2
                        ...
                        go=2 ph31 cpd2:f2
                        MCWRK  do:f2 wr #0 if #0 zd ip1 MCWRK ip29
                        lo to LBLSTS2 times 2
                        MCWRK  id0
                        lo to LBLF2 times ST1CNT
                        MCWRK  rd0  MCWRK  ip5
                        lo to LBLSTS1 times 2
                        MCWRK  id10
                        lo to LBLF1 times ST2CNT
                        exit
```

If you reverse the acquisition order of this pulse program, i.e. if you specify:

```
        aqseq 321
```

you have to change the mc clauses to:

```
         F1PH(rd10& ip1 & ip29, id0)
         F2PH(ip5, id10)
```

5.3 Additional mc clauses

Apart from the mc clauses specified above two further clauses are available:

- F1I
  this clause is typically used for interleaved experiments where
  parameters have to be varied independently from the ip/id scheme
  required for the actual 2D.

- F0
  this clause is used when a parameter needs to be varied without
  incrementing the data file pointer.

Both F1I and F0 expand to an additional inner loops.

As an example of the F1I clause, we will take the pulse program *noesygp-phprxf;* with FnMODE[F1] = States-TPPI:

```
1 ze
 d11 pl12:f2
2 d11 do:f2
3 d12 pl9:f1

   ...
   go=2 ph31 cpd2:f2
 d11 do:f2 mc #0 to 2
   F1I(ip3*2, 2, ip13*2, 2)
   F1PH(ip4 & ip5 & ip29, id0)
   exit
```

will expand to

```
"ST1CNT = td1 / ( 2 * 2 * 2 ) "
"MCWRK  = 0.166667 *  d11"
"MCREST = d11 -  d11"
          1      ze
                 d11 pl12:f2
          2      MCWRK  do:f2
LBLF1I1,         MCWRK
LBLF1I2,         MCWRK*3
```

```
LBLSTS1,     MCWRK
  LBLF1,     MCREST
         3   d12 pl9:f1
             ...
             go=2 ph31 cpd2:f2
             MCWRK do:f2 wr #0 if #0 zd ip3*2
             lo to LBLF1I1 times 2
             MCWRK  ip13*2
             lo to LBLF1I2 times 2
             MCWRK  ip4 MCWRK ip5 MCWRK ip29
             lo to LBLSTS1 times 2
             MCWRK  id0
             lo to LBLF1 times ST1CNT
             exit
```

The pulse program line below shows how the F0 clause can be used:

```
d1 mc #0 to 1 F0(id9) F1QF(id0)
```

will be expanded to:

```
...
d1*0.5 id9
lo to 2 times td0
d1*0.5 wr #0 if #0 zd id0
...
```

As a loop counter, the parameter TD0 is evaluated.

In order to be able to switch dimensions, timing of statements within the loops must be controlled by the mc statement. So delays or pulses should not be used as argument to the F0, F1PH ... clauses of the mc statement. But in some cases statements must be separated by an delay. Precautions have been taken for this case: the & symbol used within an argument of F0,... will be substituted by an equal fraction of the delay with which the mc statement was specified, e.g

```
d1 mc #0 to 1 F0(ip1 & ip3)
```

will expand to

```
MCWRK ip1 MCWRK ip3
lo to 3 times td0
```

For 3D pulse programs, the clauses F1I and F2I are available for the two

indirect dimensions.

5.4 General syntax of mc

The syntax for the mc statement is

        label <delay1> <options>
            ...
            ...
        <delay2> <options> mc #<buffer> to <label>
            F0(<statements>)
            F1I(<sts>,<no. of loops>,<sts>,<no. of loops>, ...)
            F1PH(<statements>,<statements>)
            F1QF(<statements>)
            F1EA(<statements>,<statements>)
            F2I(<sts>,<no. of loops>,<sts>,<no. of loops>, ...)
            F2PH(<statements>,<statements>)
            F2QF(<statements>)
            F2EA(<statements>,<statements>)

The following rules hold:

- <label> must be followed by one delay and can be followed by options
- <delay1> must be greater than or equal to <delay2>
- multiple clauses like F0(), F1PH(),.. can be specified on the same line or on consecutive lines. Do not specify any other statements between the clauses.
- The order in which F0(), F1PH(),... clauses occur is irrelevant
- In 3D, the statement aqseq 312 determines the order of the F1 and F2 loop
- The pulse program must contain a ze statement after the parameter definitions.
- The symbol & is required between multiple statements of the same type (e.g. multiple phase increments) that are specified within one argument.

After expansion, each statement will appear with a separate delay (see the example in section 5.3). Multiple statements of a different type (e.g. a phase increment and a delay increment) can be specified with a & symbol or with a white space in between. In the latter case, after expansion, they will appear together behind one delay.

Table 5.2 shows, which expansions will be done for different values of FnMODE.

FnMODE	create a double loop	delay-increment div. by 2	phase reset	phase inc inserted	delay inc in inner loop
QF					√
QSEQ	√	√	√	√	√
TPPI		√		√	√
States	√		√	√	
States-TPPI	√			√	
EA	√			√	

Table 5.2 Results of use of different FnMODEs

Note the following things when you view the expanded pulseprogram:

- MCWRK is a fraction of <delay2> and is calculated according to the number of arguments of the mc clauses
- MCREST is the difference between <delay1> and <delay2>
- the generated labels have names like LBLF*. Please do not use labels with these names in your own user-defined pulse programs.
- a line starting with # is a comment to the statement(s) that follow it. The comment contains the respective line number in the original pulse program, and, if applicable, the expansions that were made.

5.5 Enhancements of the mc Syntax

While in traditional nD acquisition each plane is measured completely before the next plane begins, there are new techniques where planes are not measured completely and in various orders. The new techniques are described by the parameter FnTYPE where FnTYPE="traditional" stands for the conventional technique, FnTYPE="full(points)" stands for a technique where all 2^{n-1} FIDs belonging to a complex point of an nD acquisition are measured together. For this kind of acquisition the conventional form of the mc command is no longer sufficient. Instead, the increments of the incrementable delays and the phase programs must be calculated fom the indices of the complex point in each dimension. For this purpose 2 new commands are available which can be used to calculate these increments:

calph(phX, increment) calculates the phase program increment and

caldel(dX, increment) calculates the delay which is necessary for a set of indices. An example from a 3D pulse program illustrates this:

Conventional pulse program:

    F1PH(ip5, id0)
    F2PH(rd0 & rp5 & ip7 & ip9, dd10 & id20 & id30)

Using the the new syntax the same is expressed as

    F1PH(calph(ph5), caldel(d0))
    F2PH(calph(ph7) & calph(ph9, caldel(d10, -in10) & caldel(d20) & caldel(d30))

The second argument of calph and caldel describes the increment, for calph it is the increment of the phase program in degrees, for caldel it is the increment of the delay in sec. The argument can be omitted, in this case it defaults to 90° for phases and for delays to the IN parameter of the delay specified in the first argument (IN0 for d0 etc.).

One can see that the new form of the command needs less arguments than the conventional one since it is no longer necessary to reset delays and phase programs.

Each FnTYPE requires a different kind of processing. The new mc syntax is compatible for all FnTYPEs and no modification in the pulse program is

necessary if different FnTYPEs are used.

Subroutines

5.6 Definition

A subroutine definition can be in the header of a pulse program or in an include file. It consists of the keyword subroutine and the subroutine name followed by the argument list in parentheses and by the subroutine body in curly braces:

```
subroutine SR1(<arguments>)
{
    <subroutine body>
}
```

A class name may optionally be appended to the subroutine name. This serves to identify the subroutine and to prevent it from illegal usage:

```
subroutine SR1:CLASS1(...)
```

The subroutine parameters can be pulses, delays, phase programs, loop-counters, channel specifications, gradients etc.. The name of a parameter may be any name which is not reserved in the pulse program language. The parameter types are checked as far as they are known.

```
subroutine SR1:CLASS1(pulse px, channel fx)
{
  px:fx ; a pulse with a channel in a subroutine
}
```

Subroutine calls within subroutines are possible.

Labels in subroutines are local to this subroutine and may be used by loops within the same subroutine.

5.7 Subroutine Execution

A subroutine is called with the keyword subr:

    subr SR1:CLASS1(p3, f2)

This call together with the definition in the previous section will generate the code

    p3:f2

If subroutines are defined with a class specification, it is mandatory that the same specification is added to the call of the subroutine. If labels are specified, the pulse program compiler changes them into unique names to avoid multiple definitions.

5.7.1 Subroutines with Variable Names

Different subroutines can be called from a pulse program without changing the pulse program itself by using the parameters SUBNAM1-16:

    subr <$SUBNAM1>(p3, f2)

The compiler will insert the subroutine whose name is in SUBNAM1 at this place.

The precompiled pulse program *pulseprogram* in the raw data directory always shows the expanded subroutine together with lines which mark its begin and end.

Chapter 6

Miscellaneous

6.1 Multiple receivers

If your spectrometer is equipped with multiple receivers, you can specify in the pulse program which receiver you want to use to acquire the data. The receiver number (1-8) can be appended to the following statements:

go, gonp, gosc, goscnp, adc, rcyc, rcycnp, eosc, eoscnp, ze, zd, st, st0, aq, dw, dwov, recph, wr, if

For example the statement:

go5=label

acquires the data with receiver 5

If no number is specified, 1 is assumed, i.e. go is equivalent to go1):

Parameters for the first RCU are taken from the current dataset. Parameters for the nth RCU are taken from data set n-1 of the data set list DSLIST.

The following parameters are taken from the dataset in the DSLIST dataset:

AQ_mod, DECIM, DIGMOD, DIGTYP, DR, DSPFIRM, DSPFVS, FTLPGN, NBL, OVERFLW, SEOUT, SFO1, SW, SW_h, TD.

All other parameters are taken from the current dataset.

The command *wr*n, of course, then writes out the data of this n-th RCU to the dataset n-1 of the dataset list.

6.2 Real time outputs

The spectrometer TCU provides a number of real time outputs which are used to control various spectrometer components, such as gating and blanking the transmitters. Please refer to your hardware documentation to find out which output is connected to a particular device. The pulse program compiler will select the correct output automatically, e.g. for a statement like p1:f2.

The file *$XWINNMRHOME/exp/stan/nmr/lists/pp/Avance.incl* contains a number of macro definitions based on the outputs, which can be used in pulse programs. This file can be viewed with the command **edpul Avance.incl**. Depending upon the spectrometer type this file can have different contents after 'expinstall'.

The hardware documentation will also inform you which of the outputs are free for special purposes, e.g. for controlling a laser from a pulse program.

6.2.1 Type 1 outputs ("NMR control words")

On AV systems, there are 3 outputs called RCP32, RCP33, and RCP34 in NMR0 and 32 outputs in NMR3 and 4, respectively. They can be enabled or disabled from the pulse program in a way illustrated by the examples below.

        1u setnmr0 | 32 ; set gradient blanking for z gradient

activates output channel 15 (using active=low logic). The channel remains active until it is explicitly deactivated, e.g. with the statement:

        1u setnmr0 ^ 32

The characters "|" (vertical bar) and "^" (circumflex) can be used to set and clear a bit in a register consisting of 3 bits. As such, several outputs can be

enabled or disabled simultaneously. For example, the statement:

    1u setnmr3 ^8^9 ; switch QNP to X

disables the output channels 8 and 9 of NMR3.

The statement setnmr must be specified behind a delay (in the above examples it is 1 msec). The minimum delay is 50 ns.

An alternative format for the setnmr command allows the input of whole words in hexadecimal:

    setnmr3 0xffff0000 ;set the high 16 bits of nmr word 3.

6.2.2 NCO control in AV I and AV II spectrometers:

The assignment of the bits in NMR0 is shown in table 6.1. Bits 0, 8 and 16

Bit #	Connector on TCU	Meaning	Destination
Bit 0-7	-	NCO1	SGU1-8
Bit 8-15	-	NCO2	SGU1-8
Bit 16-23	-	NCO3	SGU1-8
Bit 24-31	-	NCO update	SGU1-8
Bit 32	T2-A4	BLK_GRAD_X	GRASP
Bit 33	T2-A5	BLK_GRAD_Y	GRASP
Bit 34	T2-A6	BLK_GRAD_Z	GRASP

Table 6.1 Assignment of bits in NMR control word 0

are used to control which NCO is used in SGU1, bits 1, 9 and 17 for SGU2, and so on. If NCOs are switched, it is possible either to keep the phase setting of the destination NCO, or to take over the phase setting of some other NCO to the destination NCO. The second possiblity is called *phase continuous* frequency switching, the first *phase coherent.* One can control this behaviour with bits 24-31. The details are described in table 6.2. The phase of NCO1 can only be set from the accumulator, the phase of NCO2 can be set from NCO1, and that of NCO3 from either NCO1 or NCO2. Different bits can be combined, but, of course, it is not possible to set the phase of

NCO3 to that of NCO2 and NCO1 at the same time. Examples:

```
d1 cw:f1
d1 setnmr0|8 ; set to NCO2, keep the phase of NCO2
d1 setnmr0^8|0 ; set back to NCO1 frequency
d1 setnmr0|8^0|26 ;switch to NCO2, use the phase of NCO1          ; for
NCO2
```

This example refers to F1. If the same should be achieved on F2, the corre-

Bit #	Source NCO	Destination NCO
24	NCO2	NCO3
25	NCO1	NCO3
26	NCO1	NCO2
27	Accumulator	NCO1

Table 6.2 Phase coherence setting

sponding bits for this channel 1, 9 and 17 have to be used instead of 1, 8 and 16.

6.2.3 NCO control for AV III spectrometers

For AV III the control of the NCOs has been simplified and put together into the reset command. Reset of each NCO in each channel can be done individually. Different reset commands for different channels can be combined:

```
reset:f1:f2 ; reset all NCOs on channel f1 and f2
reset1:f2 reset4:f3 ; reset NCO1 on channel f2 and NCO3 ;from NCO2 on
f3
```

Command	Action
reset	set accumulator to 0, reset NCO1, 2 and 3 from accum.
reset1	reset NCO1 to 0
reset2	reset NCO2 to 0
reset3	reset NCO3 to 0
reset4	reset NCO3 with phase from NCO2
reset5	reset NCO3 with phase from NCO1
reset6	reset NCO2 with phase from NCO1
reset7	reset NCO3 from NCO2, reset NCO2 from NCO1
reset8	reset NCO3 and NCO2 from NCO1
reset9	reset NCO1 from accumulator
reset10	reset NCO2 and NCO1 from accumulator
reset11	reset NCO3 from NCO2, NCO2 and NCO1 from accum.
reset12	= reset

6.2.4 Real Time Pulses RTP

The real time outputs are used for the control of the digitizer. They are set implicitly with the go command in pulseprograms. If an explicit control is needed, the command setrtp<channel>|<bit>^<bit> can be used. Its usage is analogous to the setnmr commands. Table 6.4 describes the assignment of these bits for AV I and II, Table Figure 6.3. The whole register can be set with

setrtp<channel> 0x<number>

6.2.5 Fast Real Time Pulses FRTP

Each SGU has 4 FRTP outputs. They can be set with the command

Bit	symbolic name	action
0	RTP_DWELL_ENABLE	switch dwell enable on/off
1	RTP_INTERLEAVE_INCR	turn on/off interleave increment pulse for RX and HPPR
2	RGP_HPPR	switch off/on receive mode of HPPR
3	RGP_RX	switch off/on receiver blanking
4	RGP_ADC	turn off/on digital ADC blanking
5	RGP_PAUTO	turn on/off receiver (ADC, RX, and HPPR)
6	RGP_HD	enable homodecoupling

Table 6.3 : real time pulses for AV III

Bit #	Name	Meaning
0	RGP_ADC	ADC gating pulse
1	RGP_RX	Receiver gating pulse
2	RGP_HPPR	Preamplifier gating pulse
3-5	reserve	
6	interleave	selector for switching receiver and HPPR
7	DWL_CLK	dwell time for receiver ADC
8	ADC_SEL0	selects HADC/2 and SADC, resp.
9	ADC_SEL1	selects FADC

Table 6.4 real time pulses for AV I and AV II

setfrtp<channel>|<bit>^<bit>

The syntax is analogous to the setnmr command. Bit 1 is used for the amplifier blanking of the amplifier to which the SGU is routed. The blanking information is routed in the same way as the frequency. (see *edasp* command and parameter RSEL). Bit 2 is used to control the NCO selection of another SGU (used in bandselective homodecoupling experiments).

For AV III a different meaning of the bits has become necessary. The receiver gating pulses RGP_ADC, RGP_RX and RGP_HPPR are generated automatically from one gating pulse called RGP_PAUTO. The individ-

ual setting of these pulses is not possible.

6.3 Gradients

The term gradient refers to a magnetic field gradient that is added to the homogeneous field of the spectrometer magnet. A gradient is supplied by a gradient coil and can be applied in the x, y and/or z spacial dimension. If a gradient is applied in the x-dimension, the magnetic field will be constant within a y-z plane. In the y-z plane through the center of the receiver coil, the x-gradient field is zero. In a y-z plane at one edge of the receiver coil the x-gradient field is +M, whereas in a y-z plane at the opposite edge it is -M. Here, M is the maximum gradient strength which depends on the gradient amplifier. For y and z-gradients, the same principle holds concerning the x-z plane and x-y plane, respectively.

A rectangular gradient has a constant strength during the time it is applied, whereas a shaped gradient has a variable strength.

6.3.1 Rectangular gradients

A *rectangular* gradient has a strength that is constant during its execution. It can be created with one of the statements gron0, gron1, ..., gron31. The statement gron0 creates a gradient whose strength is determined by the parameters GPX0, GPY0 and GPZ0. Similarly, gron1 creates a gradient whose strength is determined by the parameters GPX1, GPY1 and GPZ1etc. The groff statement switches off all gradients that were switched on by a gron* statement.
For example, the pulse program section:

```
300u gron2
1m
100u groff
```

switches on a gradient defined by GPX2, GPY2 and GPZ2, at the beginning of a 300 msec delay. This gradient remains on during a period of 1.3 msec.

The parameters GPX0, GPY0 and GPZ0 can be set by entering *gpx0*, *gpy0*, *gpz0*, respectively, on the command line. As the gradient strength is expressed as a percentage of the maximum strength, it takes a values

between 0 and 100. The parameter, GPX1, GPY1, GPX2 etc. can be set from the command line in a similar way. Alternatively, you can set all gradient parameters from the **eda** window by clicking the *GP031 edit* button.

6.3.2 Shaped gradients

A *shaped* gradient has a strength that varies during its execution. The gradient strength as a function of time is called the gradient shape. It is defined by a list of values between -1.0 and 1.0. The number of values in the list defines the number of time intervals. Each element in the list defines the relative gradient strength during a particular time interval. The interval length is defined by the length of the entire gradient shape divided by the number of intervals. The length of the shape (duration) must be specified in the pulse program The gradients are reset to zero at the end of the shape, if no gradient statement is immediately following.

The following 3 examples generate shaped gradients:

> 10mp**:**gp2
>
> p1**:**gp1
>
> gradPulse*3.33**:**gp3
>
> vp**:**gp4 ; Incorrect! Shaped gradients with vp are not supported.

They are applied for 10 millisec, P[1], and gradPulse*3.33 and are described by the *gradient parameter table* entries 2, 1, and 3, respectively. This table can be opened by clicking on the *GP031* button in **eda**. It has 32 entries with indices 0-31. The statements **:**gp0 interprets entry 0, **:**gp1 interprets entry 1, etc.

Each entry of the gradient parameter table has 4 assigned parameters: *GPX, GPY, GPZ* (the gradient strength multipliers for the 3 spatial dimensions), and a *file name* (of the file that contains the gradient strength values).

GPX, GPY, GPZ
These are multipliers with values between 0 to 100. They are applied to the gradient strength values (which range from -1.0 to 1.0) in the shape file to obtain the total gradient field strength.

File name

File name is the name of a gradient file. A gradient file can be generated from Shape Tool window (command **stdisp**) or from the command line with the command **st** (for more information click **Help** ' **Online Manual** from the Shape Tool window).

Gradient shape files are stored in JCAMP-DX format in the directory:

> *$XWINNMRHOME*/exp/stan/nmr/lists/gp/

Note that if you specify an internal gradient shape, you don't need a shape file, however you should define the length of the shape as described below.

All gradient parameters can be set from from the **eda** window by clicking the *GP031 edit* button. Alternatively, they can can be set by entering **gpx0**, **gpy0**, **gpz0**, **gpnam0**, **gpx1** etc. on the command line. As the gradient strength is expressed as a percentage of the maximum strength, it takes a values between 0 and 100.

As described in the next section, you can also define gradient shape functions in the pulse program rather than using shaped gradient files.

6.3.3 Gradient Functions

You can use gradient shapes as gradient functions. Then the current function value is used to calculate the gradient.

Shaped gradients can be defined in the pulse program as a gradient function. At each moment, the gradient strength is set to the current function value.

The function index can be manipulated with the following statements:

```
zgrad sin ; zero index -> use 1st function value
igrad sin  ; increment index
dgrad sin ; decrement index
sgrad sin ; save index (stack with depth = 1)
rgrad sin ; restore index

sgrad sin ; save the current index
rgrad sin ; restore the last saved index
```

The length of an internal gradient function (or shape) must be specified at the beginning of the pulse program, e.g.:

lgrad sin = 100; sine function with 100 values

Internal Gradient Functions:

A gradient function is either a gradient shape that is defined in a gradient file, or an internal function that is calculated during pulse program compilation. The following internal functions are available:

- *plusminus*
  can take the value 1 or -1.

- *r1d*, *r2d* and *r3d*
  linear ramps from -1 to 1, where the final value is never reached.

- *step*
  linear ramp from 0 to 1 and the final value will always be reached.

- *sin*
  sine function from 0 to p (excluding p). The angle increment depends on the length of the function (see above).

- *cos*
  cosine function from 0 to p (excluding p).

- *sinp*
  sine function from 0 to p (including p).

- *gauss <truncval>*
  which is a gaussian function with truncation level (e.g. gauss2.5 for 2.5% truncation level)

- *rnd*
  random function.

6.3.4 Manipulation of rectangular or shaped gradients

Both rectangular and shaped gradients can be manipulated with a constant and/or a gradient function. Here, manipulation can be addition or multiplication.

Example:

```
1 300m gron2 * - 0.5 * plusminus
p1 gp1 * sin(100) * cnst0
igrad plusminus
igrad sin
```

lo to 1 times 100

If a rectangular gradient is manipulated with a gradient function, the latter must be specified without parameters. For example:

300m gron2 *sin

If, however, a shaped pulse is manipulated with a function, the latter can be specified with or without parameters. For example:

p1 gp1 * sin

p2 gp2 * sin(100)

6.3.5 General Gradient Statements

Since the TOPSPIN gradient software is also used by ParaVision, it has features, that actually designed for medical imaging. With gradient statements of the form:

delay grad{<1st dim> | <2nd dim> | <r3d dim>}

you can use these features even without ParaVision, but in a restricted manner:

- You can specify *Object Oriented Gradients,* that are converted into *Physical Gradients.* This allows for:

  - Acquisition of images with different *slice orientation* while using the same pulseprogram. The gradients may be specified in spatial coordinates other than x, y and z. The pulse program compiler multiplies the gradients with a *rotation matrix* (see below) to get x, y and z.

  - Acquisition of images with different *slice thickness* and *field of view*, every spatial dimension may be multiplied by a *scaling factor*.

- The gradients are defined as a percentage *of maximum_gradient strength*, as *scalar values* or *functions*, which may be combined by *addition* and *multiplication*.

- The functions are either *Internal functions*, which are handled accordingly by the compiler, or *gradient files* containing the function values (see above).

- Scaling and rotation can be suppressed with the following options:

no_scale: Gradient is not scaled

direct_scale or *shim_scale*: Gradient is not scaled and not rotated

- Hardware dependencies can be accounted for by specifying different values for xyz.

Examples:

10u grad{(0)|r2d(100)|(0)}; Ramp in the 2nd (or phase) dimension.

1m grad{sin(50,200)*r3d(89|90|91)+cos(50,200) | (20)|(2|1|3,direct_scale)}

The 1st (or read) dimension contains *sin(50,200),* that means: a *sine* function with 50 % amplitude. The 2nd parameter indicates a gradient shape, consisting of 200 values, every value applied 1/200 ms = 5 us.

Every *sine* value is multiplied with the current value of *r3d(89|90|91)*. The amplitude of *r3d* is different for xyz to account for hardware dependencies.

The 1st dimension also contains a 2nd gradient shape *cos(50,200)*. You can combine several gradient shapes in one statement, but the same length should be used.

The 2nd (or phase) dimension contains *(20)*, indicating a scalar gradient with 20 per cent amplitude.

The 3rd (or slice) dimension contains *(2|1|3, direct_scale)***,** indicating a sca-lar gradient with 2 per cent amplitude in x direction, 1 per cent in y and 3 per cent in z, independent of rotation and scaling.

6.3.6 Rotation and Scaling

If the EXPNO directory of the current data set contains a text file cag_par, the
rotation and scaling is done, as specified in this file.

Else if $XWIN-NMRHOME/exp/stan/nmr/lists/gp contains a text file cag_par, the rotation and scaling is done, as specified in this file:

Example:

0.5   ; Scaling of 1st (or read) dimension

| 0.5 | ; Scaling of 2nd (or phase) dimension |

| 0.8 | ; Scaling of 3rd (or slice) dimension |

In this case you can acquire 2 slices with different orientation. Like function indices, you can manipulate slice indices with the statements zslice, islice, dslice, sslice, rslice.

1.0	0.0	0.0	;	Scaling of 1st (read or x) dimension
0.0	1.0	0.0	;	Scaling of 2nd (or y) dimension
0.0	0.0	1.0	;	Scaling of 3rd (or z) dimension
1.0	0.0	0.0	;	1st rotation matrix
0.0	1.0	0.0		
0.0	0.0	1.0		
0.707	0.707	0.0	;	2nd rotation matrix
-.707	0.707	0.0	;	the 1st and 2nd dimensions are rotated by
0.0	0.0	1.0	;	45 degrees

Table 6.5 example of a cag_par file

6.4 Miscellaneous statements

6.4.1 Switching on/off Presetting of Blanking Pulses: preset

The preset off statement switches off the presetting of blanking pulses. The program will then behave as if all *preset* parameters (command **edscon**) are set to 0. Switching of the presetting must occur at the beginning of the pulse program and can not be undone.

6.4.2 Assignment of Transmitter Blanking Pulses: blktr

The transmitter blanking pulses are normally set by the **edscon** preset parameters (BLKTR[1...8]). They can, however, also be declared at the

beginning of the the pulse program using the syntax:

blktr<channel number> = <duration>

Example:

"blktr1=3u"

NB: for AV I and II the assignment of the BLKTR parameters to channels is different to those of AV III. In the former the assignment was a logical assignment, i.e. if F1 controlled SGU2 and from there amplifier 3, BLKTR1 was applied to channel F1 and in this way to amplifier 3, whereas in AV III BLKTR is always applied to the amplifier with the same number (which is determined by the blanking signal of this amplifier).

6.4.3 Generation of Blanking Pulses: <u>gatepulse</u>

Blanking pulses are automatically generated according to the ***edscon*** pre-set parameters. If, however, the pulse program contains the statement pre-set off the generation of blanking pulses is disabled. In that case, you can selectively enable the generation of blanking pulses on a particular channel. This can be done with the gatepulse statement. The syntax is:

delay gatepulse 1 [| 2...]

Example:

3u gatepulse 1 ;generate blanking pulse for f1
p1:f1
d1
2u gatepulse 1|2 ;generate blanking pulses for f1 and f2
(p1):f1 (p2):f2

Note that gatepulse statement will only generate the blanking pulse for the transmitter, the preamplifier and the ASU.

6.4.4 Printing messages

The statement

print "Hello World"

prints the message *Hello World* during runtime of an experiment. The timing of the printout follows the interpretation of the pulse program on the TCU and may be therefore ahead in time of the execution of the pulse pro-

gram. However, for debugging complex pulse programs it could be helpful.

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