

# Fourier

- Fourier 300  
Quick-Start Installation Guide  
Version 001



Copyright© by Bruker Corporation

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form, or by any means without the prior consent of the publisher. Product names used are trademarks or registered trademarks of their respective holders.

This manual was written by

Diether Maier

© December 20, 2011: Bruker Corporation

Rheinstetten, Germany

P/N: Z33048

DWG-Nr.: Z4D11877

For further technical assistance on the Fourier unit, please do not hesitate to contact your nearest BRUKER dealer or contact us directly at:

BRUKER Corporation  
am Silberstreifen  
D-76287 Rheinstetten  
Germany

Phone:+ 49 721 5161 0  
FAX:+ 49 721 5171 01  
E-mail:service@bruker.de  
Internet:www.bruker.com

---

<b>1</b>	<b>Getting Started</b> .....	<b>5</b>
1.1	This Manual.....	5
1.2	Before You Begin.....	5
1.3	Unpacking the Console.....	5
1.4	Console Connections.....	6
1.5	External Filters.....	6
1.6	Adjusting the Air Pressure.....	7
1.7	Switching On the Console the First Time.....	7
1.7.1	Verifying That the Console Has Booted.....	7
1.8	Copying the Probe Data to the PC System.....	8
1.9	Setting the Magnet to the Correct Field.....	9
1.10	Setting the Spin Safety Threshold.....	9
1.11	Initial Shimming.....	11
1.12	Finding the Lock Field and Phase.....	11
1.13	Manual Shimming to Lineshape.....	12
1.14	Converting the Parameter Set to the Actual BF1.....	12
1.15	Creating a Shim Map for Gradshim.....	13
1.16	ATP Tests and Customer Acceptance.....	14
<b>A</b>	<b>Appendix</b> .....	<b>17</b>
A.1	Main Differences Between Fourier and AVANCE.....	17
1.2	Figures.....	19



# 1 Getting Started

## 1.1 This Manual

---

This manual is intended to be a quick-start reference guide for Bruker service technicians. It provides basic information for installing and setting up the Fourier 300 system.

**Carefully read the information in this manual, as well as, the safety information provided in the Service Manual before working on the device!**

This manual provides only the basic information required for installation and set-up, for complete information refer to the service manual.

## 1.2 Before You Begin

---

This guide assumes that the magnet has been evacuated, cooled down, and that all the equipment for energizing that magnet is available on site.

Three test samples, two spinners and a sample gauge are shipped with the system.

- 3% CDCI3 in Chloroform (lineshape)
- 0.1% EB in CDCI3 (1H SINO)
- ASTM (C13 SINO)

To shim the magnet and perform the ATPs test you will need to bring some additional samples:

- Urea in DMSO (Pulse Length adjustment)
- 100mg or 1g Cholac in CDCI3 (DEPT)
- Cyclosporine in C6D6 (2D Examples)

## 1.3 Unpacking the Console

---

**Do not attempt to lift the Fourier console out of the carton**, rather:

1. Slide the carton sleeve up and over the console.
2. Slide the console off the pallet.

The console has wheels and can be moved around freely using the handle on the back.

Retain the packaging in case the console has to be returned for repair/exchange.

## 1.4 Console Connections

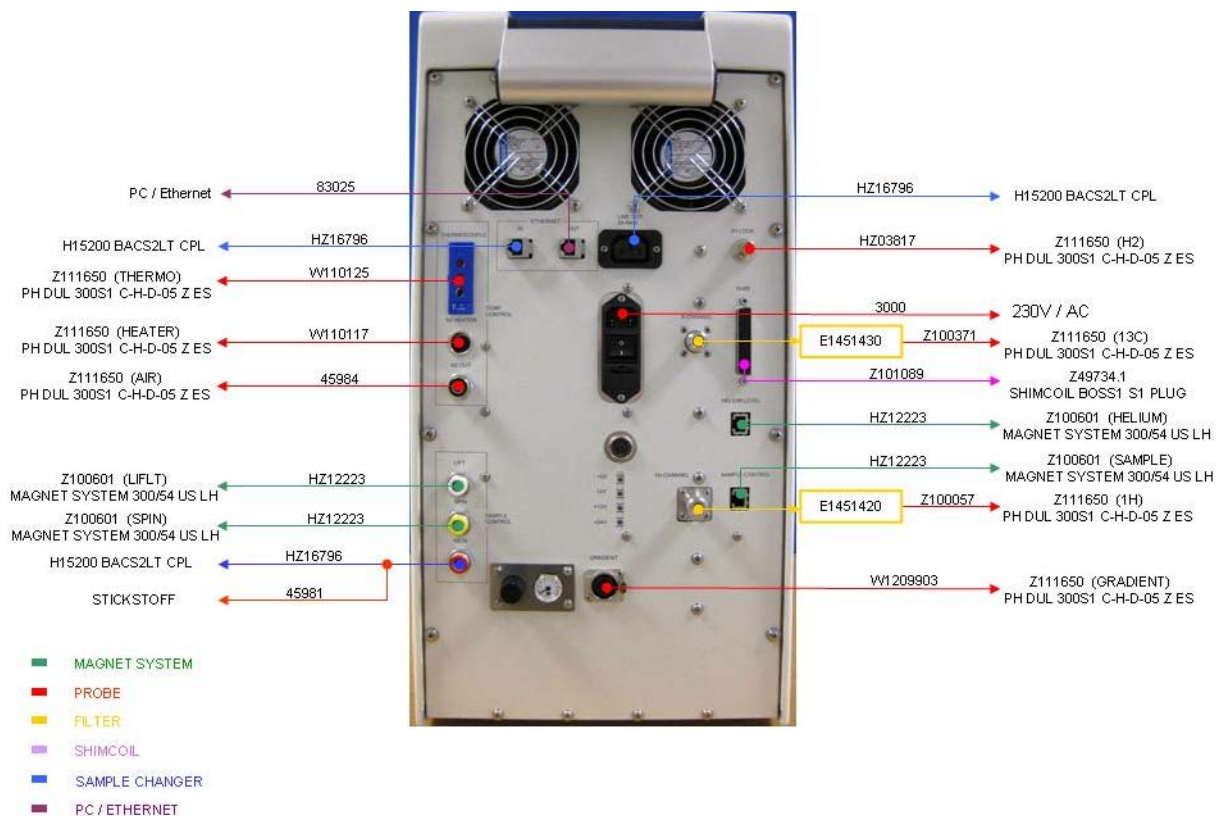


Figure 1.1 Console Connections

## 1.5 External Filters

Some earlier models come with three external filters:

- Z13383 is connected to the 1H connector on the rear of the console.
- Z14331 is connected to the C13 connector on the rear of the console.
- Z00116 is connected to the C13 connector of the probe.

Later models have just two external filters:

- E1451420 is connected to the 1H connector to the rear of the console.
- E1451430 is connected to the C13 connector to the rear of the console.

## 1.6 Adjusting the Air Pressure

Adjust the air pressure so that the manometer in the console reads between 3.5 and 4 bar. This way the default spin and lift parameters will be sufficient to get you started.

## 1.7 Switching On the Console the First Time

The console has three modes:

- OFF (blue light OFF), the switch on the rear panel is set to OFF.
- STAND BY (blue light BLINKING), the switch on the rear panel set to OFF, the ON/OFF button on the top of console is not yet pressed.
- ON (blue light ON).

It is IMPORTANT to switch the console on BEFORE switching on the PC, since the console contains the Ethernet hub, and the DHCP server will not start if a network is not found.

### 1.7.1 Verifying That the Console Has Booted

This procedure takes 30-60 seconds, provided the DHCP server is already running. There is no visual indication on the console indicating that the console has booted, but the easiest way to check is to see if the three main Ethernet devices (main board, lock and VTU) can be reached via ping or a Web browser. Their addresses will usually be in the range:

149.236.99.25x

To access any of the Web server sites, the following password and user name are required:

User: **root**

Password: **BRUKER** (in capitals!)

If you are not sure the DHCP Server is running, you can check by opening:

**Control Panel -> Administrative Tools -> Services -> Bruker DHCP Server**

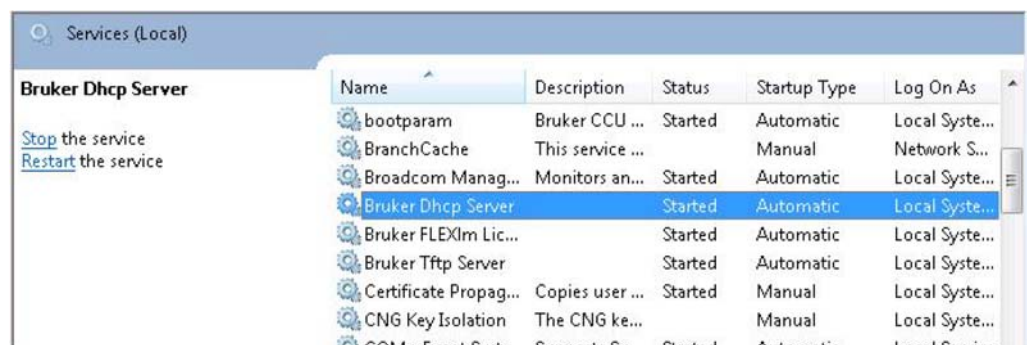


Figure 1.2 Bruker DHCP Server

If you are not sure what addresses have been assigned, you can check by opening the following file:

Bruker\Diskless\dchpd.leases

```
lease 149.236.99.254 {
starts 4 2010/08/19 11:08:55;
ends 2 2038/01/19 03:14:06;
tstp 2 2038/01/19 03:14:06;
binding state active;
next binding state free;
hardware ethernet 00:00:ad:11:4f:12;
uid "\001\000\000\255\0210\022"; }
```

```
lease 149.236.99.253 {
starts 4 2010/08/19 11:08:58;
ends 2 2038/01/19 03:14:06;
tstp 2 2038/01/19 03:14:06;
binding state active;
next binding state free;
hardware ethernet 00:00:ad:13:34:12;
uid "\001\000\000\255\0234\022"; }
```

```
lease 149.236.99.252 {
starts 4 2010/08/19 11:09:01;
ends 2 2038/01/19 03:14:06;
tstp 2 2038/01/19 03:14:06;
binding state active;
next binding state free;
hardware ethernet 00:00:ad:12:85:12;
uid "\001\000\000\255\022\205\022"; }
```

Once you are sure that all three devices have booted, you can start TopSpin. Normally, the PC will come with the hardware configuration (CF) having already been carried out. If you receive an error message stating that one or more devices cannot be found, you may have to repeat CF (refer to Chapter 9 of the NMR Experiments User Manual).

## 1.8 Copying the Probe Data to the PC System

---

Since the Fourier system always comes with the same type of probe, there is no PICS interface on the Fourier console. Instead a CD-ROM with the probe data is delivered with the system. Before running EDHEAD, copy the probe.ph file from the CD-ROM to the directory:

**“conf/instr/FOURIER300”**

## 1.9 Setting the Magnet to the Correct Field

---

The magnet is designed to be operated at **300.18 MHz**, with the current in the H0 field coil of the shim system set to zero. At this frequency the synthesizers are “cleanest” and least likely to create spurious problems.

When the lock is powered up from a cold start, **the field DAC is not automatically set**. In order to make sure the current in the field coil is set to zero:

1. Open the BSMS panel.
2. Set the field value to 2048.
3. Switch the lock to “ON” once, then switch it off again while the magnet is being charged to the correct field and the cryo-shims are adjusted.

## 1.10 Setting the Spin Safety Threshold

---

The spin has a safety function that shuts the spin off as soon as the Lift is turned on, either manually, or during the initialization of the sample changer. In order to do this, the analog sensor that monitors the spinner has to be calibrated. The sensor has three voltages for the three possible states:

No spinner (typically 0.1 to 0.6V)

Black (typically 0.6 to 1.5V)

White (typically 2.5 to 4.5 V)

Since the values vary between shim stacks, and also depend somewhat on the spinner type, it is necessary to calibrate this value. Usually this only has to be done once at installation.

1. Open the Web server of the VTU and go to -> peripheral control -> spin

**Spin:**

Spin frequenz:  Start Set Spin frequenz[Hz]

Stop

Get Spin frequenz

Get Spin Voltage

Spin DC Voltage Counter	<input type="text" value="10"/>
Sample Down Threshold Voltage	<input type="text" value="0.35"/>

Figure 1.3 Setting the Spin Safety Threshold

2. Remove the sample, or activate the sample lift, and annotate the “empty” spin voltage.
3. Insert, or lower the sample, and switch on the spin (either from the BSMS panel or from the Web server).
4. Repeatedly read the spin voltage and annotate the two values that can be read while the sample is spinning.
5. Set the “sample down threshold voltage” to about halfway between the lower of the two “black/white” spin voltages, and the “empty” spin voltage.

Everything is set correctly when the spin does not cut off during normal operation, but cuts off immediately when the lift is activated.

**Note:** The “Spin DC Voltage Counter” sets the number of times the value has to be below the threshold, before the safety shut off is activated. It should be set to 10 to avoid the spin cutting off with just a single bad reading.

## 1.11 Initial Shimming

First level shimming is done in the usual way by first setting the currents given in the magnet manual and then seeing if the base shim can be improved in the GS mode.

Once the cryo-shims are set, continue adjusting the lower orders of the BOSS1 shim system in the GS mode until your FID half height has reached approximately 100 ms.

## 1.12 Finding the Lock Field and Phase

Once your shim has reached a certain level, your lock should begin to show a signal.

1. Enable the Lock sweep mode in the BSMS panel.
2. Adjust the field and phase such that the “wiggles” are centred around zero and the first wiggle is positive in both directions.

Due to sidebands, there will be more than one lock field value that gives a lock signal. You can check which is the correct one by making a measurement, and checking that the spectrum has the correct ppm scale (e.g 4.7 ppm for water, 7.2 ppm for a C6D6 solvent peak).

Alternatively, you can use the Fourier AU program “flock”, which queries for the lock solvent, creates a temporary 2H data set and starts an acquisition to find the lock signal in the 2H spectrum. Flock compares the ppm shift of the 2H signal to the default value from the edlock table. The difference in ppm is then converted to a shift in the lock field. The new lock field is displayed in a pop-up window. Additionally, flock informs the operator how many solvent peaks have been found and if this number is in agreement with the number of resonance lines for the selected lock solvent. When the number of signals is different from the expected value, flock uses the peak with the highest intensity to calculate the lock shift. The new shift value is set in the Fourier and a normal lock procedure is started.



Figure 1.4 Results of the AU Program FLOCK

The flock command also works with solvents with more than one peak and can be fine tuned. Refer to the service manual for details.

Any time, the lock field changes by a large amount, the following message is shown:



Figure 1.5 Updating the BSMS Field Value in the edlock Table

Pressing OK updates the BSMS field value in the edlock table. A subsequent lock procedure should be able to find the lock signal in the usual way.

## 1.13 Manual Shimming to Lineshape

---

Follow the usual procedure, referring to the Fourier NMR Experiments User Manual when more information is needed.

Since the shimming process may have an effect on the B0 field, it may be necessary to redefine BF1 after shimming and lock have been optimized. The ideal BF1 is close to 300.18 when the lock field DAC is close to 2000 ( $\pm 500$ ).

## 1.14 Converting the Parameter Set to the Actual BF1

---

Before converting the parameter set, make a backup copy of the PAR directory, e.g:

```
C:\Bruker\TopSpin3.1.b.12\exp\stan\nmr\par
```

This can be done using CF, followed by “expinstall”. However, the preferred way is to use CF, followed by the command “paracon”, since it also converts parameter sets in the user directory. Ignore any error messages when starting, and press “Select all” in both categories, then execute.

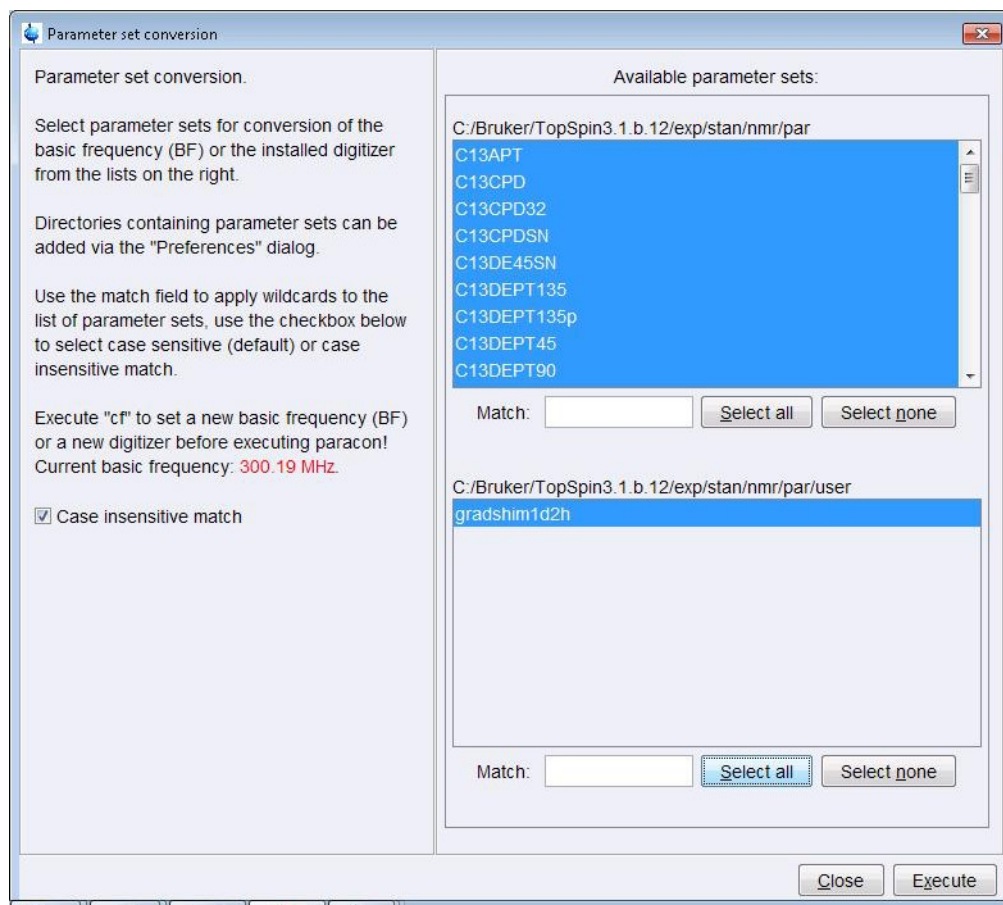


Figure 1.6 Parameter Set Conversion

**i** **NOTE:** If the BF1 has been changed, you will need to restart the console after performing CF, or paracon has been carried out. Otherwise, the lock frequency will not be updated.

## 1.15 Creating a Shim Map for Gradshim

Gradshim works best when the shim map was made using a well shimmed magnet.

Also important for the success of gradshim are that:

- The gradient echo is nicely centered in the spectral width – check by loading the experiment gradshim 1D2H.

If the gradient echo doesn't look like the figure below, it may be that the parameter sets have not been converted properly to the correct BF1.

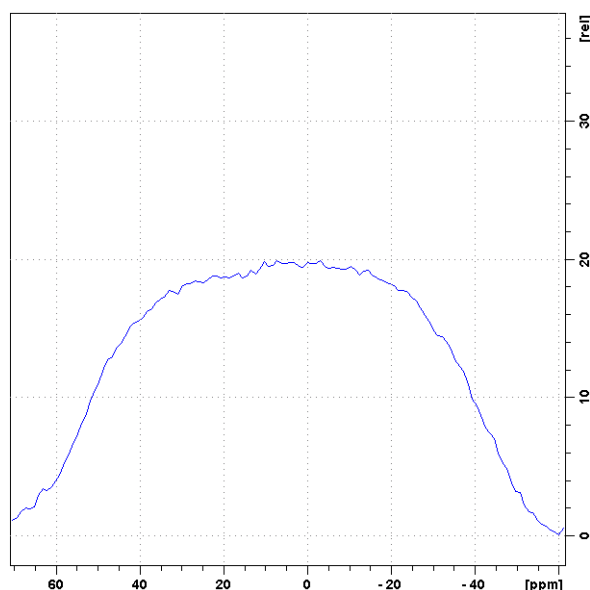


Figure 1.7 The Gradient Echo Centered in the Spectral Width

- The 2H pulse length is correct. This is normally around 50  $\mu$ s at 40 W and can be checked using a **zg** experiment, where 2H is selected as the observe nucleus. If the lock is still running when you do this, there will be spikes in the 2H spectrum!

**Important Note:**

Gradshim uses different parameters on a Fourier than on an AVANCE system. Be sure to define the parameter sets Gradshim 1d1h\_f or Gradshim 1d2h\_f when creating a shim map.

In order for gradshim to work from the “shim” button of the flow bar, and also from IconNMR, it is necessary to store the current configuration for automation (Setup -> Store for automation). The flow bar or IconNMR will call either a 1H or a 2H gradshim, depending on what was selected, when the setup was stored for automation.

## 1.16 ATP Tests and Customer Acceptance

The required **Hardware Tests (HWT)** for the Fourier 300 are carried out during console end testing and are not intended to be repeated at the customer site. The following ATP tests are relevant for the Fourier:

- Determination 90 degree 2H observe pulse
- Determination 90 degree 1H observe pulse
- Determination 90 degree 13C observe pulse
- Determination 90 degree 1H decoupling (CPD) pulse
- Determination 90 degree 1H high power decoupling pulse
- Determination 90 degree 13C low power decoupling pulse

- Lineshape test for 1H with rotation
- Resolution test for 1H
- Sensitivity test for 1H
- Lineshape Test for 13C with rotation
- Resolution test for 13C
- Sensitivity test for 13C (ASTM)
- Sensitivity test for 13C (EB)
- HSQC experiment with Z?gradient (console test)
- COSY experiment with Z?gradient (console test)
- DEPT?90 experiment
- DEPT?135 experiment

There are only three hardware specifications for the Fourier required for a customer sign off:

Lineshape using 3% CDCl <sub>3</sub> in Acetone:	0.5/8/16 Hz (non-spinning)
1H Sensitivity (0.1% EB in CDCl <sub>3</sub> ):	> 120:1 (after gradshim)
C13 Sensitivity (ASTM):	> 85:1 (after gradshim).

The remaining ATP tests implicitly demonstrate the systems remaining functions:

- Sample Spin & Lift
- Auto-Locking on various solvents
- Gradient Functionality (2Ds & Gradshim)
- Gradshim reproducibility
- Lock and Temperature Stability (COSY & HSCQ)
- Baseline & Spectral Purity (DEPT)\*

Certain artefacts are normal and have been considered acceptable for the intended use of the Fourier:

- A moderate amount of T1 noise in 2D experiments.
- Some “digital noise” on strong signals that require RG < 10. Use **zg30** instead of **zg** if that happens, in order to be able to increase the RG.
- Some vibration noise close to the feet of very narrow lines (e.g. lineshape samples). This can be improved with vibration damping if required.
- Some very small spurious spikes in the first few scans of C13 spectra. These should average out after NS > 64.
- “Asymmetric smileys” in some 1D spectra with high intensity. This can also be seen as reduction in the level of noise of about 200 Hz from the right edge of some 1D

and 2D spectra. If this part contains spectral information, simply increase the spectral width.

---

**i** **Note:** If you obtain reproducible “**spurious spikes**” in <sup>1</sup>H spectra it may be due to an unfavorable BF<sub>1</sub> frequency. The Fourier DDS are “clean” for at least 200 ppm at around 300.18 MHz.

---

# Appendix

# A

## A.1 Main Differences Between Fourier and AVANCE

The main differences between the Fourier and AVANCE are that with the Fourier:

- The lock works at 1 kHz instead of 6 kHz, which means that sidebands are closer together. Also, the lock parameters have different units for BSMS values.

Table 1.1. Typical BSMS Values for the Fourier

P:	0.1 to 0.8 depending on solvent. Higher values mean more <b>proportional</b> gain.
I:	0.1 to 0.8 depending on solvent. Higher values mean more <b>integral</b> gain.
Power:	-12 to -28 dBm depending on solvent. <b>Note:</b> The values shown in the BSMS panel are attenuations from 0 dBm.
Filter:	4 for strong solvents, 1000 for weak solvents. The numbers are not the bandwidth in Hz but the number of averages per second. A value of 1000 is equivalent to 1 Hz, 4 is equivalent to 250 Hz.
Field:	0 to 4095. A value of 2048 means no current flowing in H0 Coil. The ideal value is between 1500 and 2500, to allow for magnet drift. The BSMS field has the opposite polarity, i.e increasing the value of the field DAC by 1000 steps will cause a shift left (i.e increase the frequency) by 20 ppm.

- The shims and the BSMS field are not automatically set after power up. You will need to load a valid shim set using “**rsh**” to set the shim currents, and switch on the lock in the BSMS panel to set the current BSMS DAC value.
- The shim values range from -32768 to 32768. When converting from an AVANCE shim file, you will need to halve the values to get a good starting point.
- There is no PID self tune for the lock, VTU and spin parameters. Since the Fourier is only sold with one probe, the defaults, when operated at 4 bar, are usually good enough for all experiments. Refer to the service manual for defaults.
- There is no PICS. You will need to copy “probe.ph” to the corresponding directory.
- The “**wobb**” command doesn't work from within TopSpin. There is a wobble function using a stand-alone program. Refer to the service manual for details.
- There is a different pulse programmer language. Refer to the service manual for details.
- The Digitizer Type must be set to “DRMS”.
- The Aq.mod must be set to qsim.
- The Fn\_Mod must be set to TPPI or QF.
- The BC-Mod must always be set to OFF.
- The GPNAM must always be RECT.1.



## 1.2 Figures

---

Figure 1.1	Console Connections.....	6
Figure 1.2	Bruker DCHP Server.....	7
Figure 1.3	Setting the Spin Safety Threshold .....	10
Figure 1.4	Results of the AU Program FLOCK .....	11
Figure 1.5	Updating the BSMS Field Value in the edlock Table .....	12
Figure 1.6	Parameter Set Conversion.....	13
Figure 1.7	The Gradient Echo Centered in the Spectral Width.....	14





---

 **Bruker Corporation**

[info@bruker.com](mailto:info@bruker.com)  
[www.bruker.com](http://www.bruker.com)

Order No: Z33048

---