ATM Accessory

User Manual
Version 002

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General Description 1

Introduction 1.1

This manual describes the ATM (**A**utomatic **T**uning and **M**atching) Accessory for fixed-channel and broad-band probes. The ATM Accessory consists of hardware, which is part of the probe, and some commands in the XWINNMR software.

The ATM Accessory allows to optimize the tuning and matching automatically for each sample.

Requirements 1.2

To operate the ATM Accessory, the following hardware and software is required

1. AVANCE NMR spectrometer

2. Probehead equipped with ATM Accessory

3. Cable Z2927 connecting the PIC system module of the probe to the HPPR.

4. XWINNMR software version 2.6 or later

5. Patch with ATM software version 2.0 or later

Features 1.3

- Automatic matching and tuning of all routed nuclei
  (nucleus must be observable)

- Best performance (S/N) in automation, e.g. when using a sample changer

- Easy manual matching and tuning under software control

- Automatic nucleus change on broad-band probes

- Easy set up for new nuclei on broad-band probes

- Simple installation of probeheads equipped with ATM Accessory into the magnet without the need for mechanical adjustments

Operating Limitations *1.4*

Take care not to exceed the limitations defined in this chapter and on all documents and tags attached to the probe itself. If multiple limitations apply to your probe, the most restrictive limitation is applicable.

- General operating limitations refer to the Probes User Manual

- Sample temperature: to be defined

- Humidity max 95% (non condensing)

- When the ATM Accessory is attached to the probe, mandatory to keep the probe vertical when manipulating the tuning and matching controls by hand using the special tool. Otherwise the gearbox in the accessory may be damaged.

Abbreviations *1.5*

- PIC system   **P**robehead **I**dentification and **C**ontrol system
- ATM   **A**utomatic **T**uning and **M**atching Accessory
- S/N   **S**ignal to **N**oise
- HPPR   **H**igh **P**erformance **PR**eamplifier
- BASH   **B**ruker **A**dvanced **S**ervice **H**andbook
- XWINNMR   acquisition, processing and analysis software

Installation

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## *Inserting the probe into the magnet*   *2.1*

Inserting a probe with attached ATM Accessory, is as easy as a probe without one.

The probe will be fixed to the shim system with two screws located inside the ATM Accessory. The position of these screws is the same as for normal probes. Tighten these screws alternately without using excessive torque, by using the attached handle (shown in Figure 2.1).

High torque does not improve measurements but may damage the probe.

Figure 2.1.   Broad-Band Probe with ATM Accessory

MOUNTING SCREWS
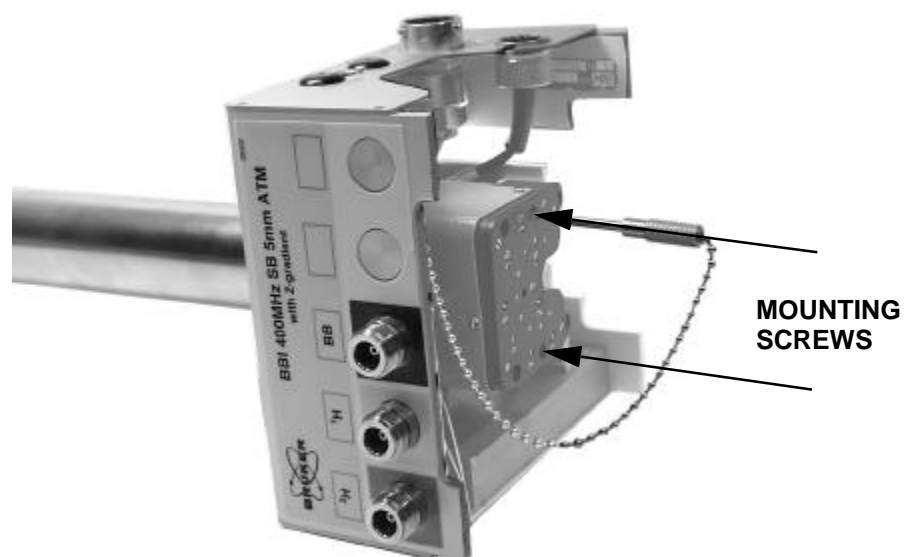
!   *In the case of a strong magnet it is possible, that the probe may be attracted. Be careful when transporting the ATM Accessory near the magnet.*

Further information about probes can be found in Probes User Manual (BASH).

Connecting the probe *2.2*

To operate the ATM Accessory a connection from the probe to the HPPR is required. Use only the cable Z2927 (HPPR/PIC System).

! *Connecting while the HPPR is running, the HPPR may reset (lamps will black out). If this happens, the HPPR must be initialize by typing the command II in XWINNMR. For further details consult the XWINNMR Software Manual*

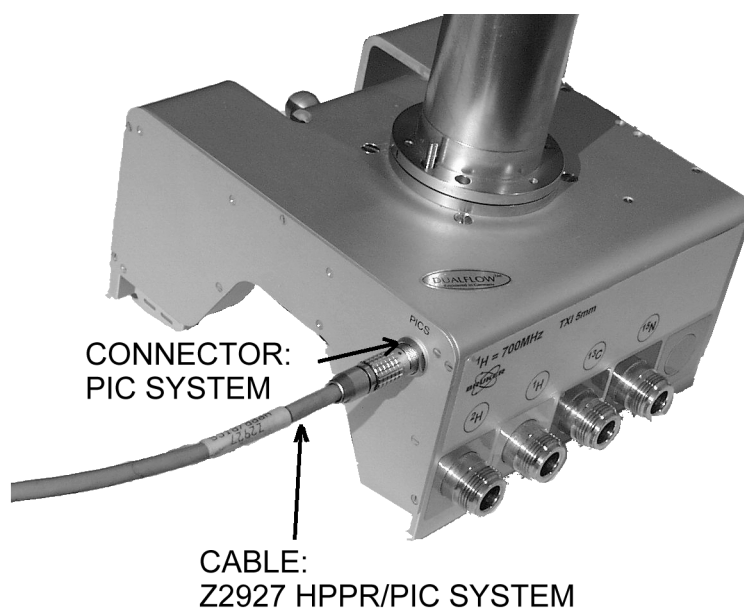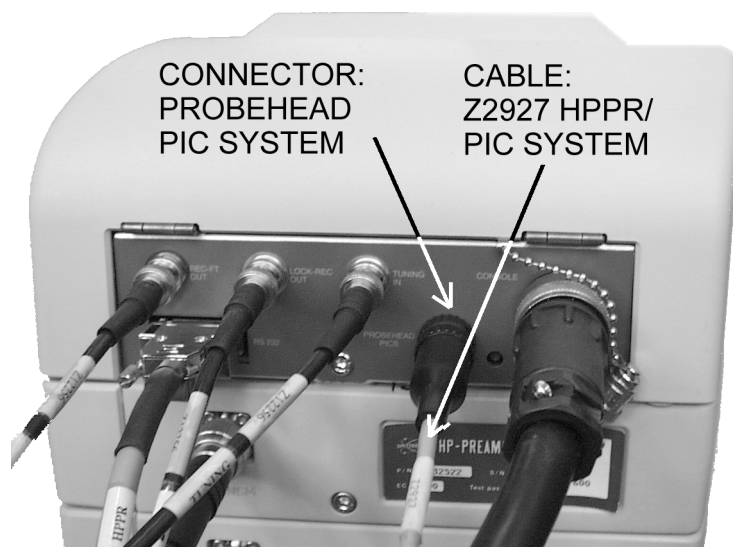*Figure 2.2. Probe with connected PIC System cable*

CONNECTOR:
PIC SYSTEM

CABLE:
Z2927 HPPR/PIC SYSTEM

Figure 2.3. HPPR with connected PIC System cable

CONNECTOR:
PROBEHEAD
PIC SYSTEM

CABLE:
Z2927 HPPR/
PIC SYSTEM

Software 3

XWINNMR commands atma and atmm *3.1*

Two new commands, **atma** and **atmm**, have been integrated in XWINNMR and are described below. Both commands relay on the **edsp** setting of the current dataset.

- The command **atma** (*automatic tuning matching automatically*) is the way to get the best performance. It will automatically tune and match your probe, without any intervention.

- The command **atmm** (*automatic tuning matching manually*) is mainly used for verifying the nuclei position on broad-band probes. It allows the positions of the tuning and matching rods of the probe to be operated directly via the workstation. A separate window will be opened showing various controls.

! *Remarks for atma and atmm:*

- Both commands, **atma** and **atmm**, will separately start the wobble procedure.

- The wobble width (**wbsw**) and the number of wobble steps (**wbst**) will be automatically defined dependent on the nucleus. After finishing of **atma** or **atmm**, the old state of **wbsw** and **wbst** will be restored. For **atmm,** user defined values can be used with the option **manWbsw**

- A special wobble procedure is started when either **atma** or **atmm** is active. It has a non equispaced frequency range and uses mostly an extended wobble sweep with. So the wobble curve may looks unfamiliar.

- **atma** will stop spinning the sample to obtain optimal results. After **atma** has finished, the old state will be restored.

- **atma** and **atmm** cannot be terminated with the **stop** command. The procedures can be terminated only with **kill**.

- **atmm** reads the reference point only at the beginning and is not updated. This can lead to large errors on the depicted wobble curve especially after a frequency change

atma process *3.1.1*

The command **atma** will automatically tune and match your probe, without any intervention

atma will do the following operations:

1. Read the probe information from the PIC system and get information of the routed channel in XWINNMR (e.g. **edsp**)

2. Turn off the sample rotation and set the optimal wobble width (***wbsw***) and the number of wobble steps (***wbst***) for the given channel

3. Set the broad-band channel on broad-band probes, to the configured nucleus. The first time after plugging in the PIC System connector, the auto configuration can take several minutes

4. Start a special wobble process to get the best resolution. The wobble curve may look unfamiliar

5. Optimize the tuning and matching in several optimization cycles

6. Stop the wobble process

7. Restart the process at step 4, if another channel must be optimized

8. Restore the old value for ***wbsw***, ***wbst*** and the sample rotation

9. Terminate the ***atma*** command with a specific status (description in chapter: Command Status). If optimization was not successful, a window with a message will be shown.

---

atmm process   *3.1.2*

The command ***atmm*** allows the positions of the tuning and matching rods of the probe to be operated directly via the workstation.

atmm will do the following steps:

1. Read the probe information from the PIC system and get information of the routed channel in XWINNMR (e.g. ***edsp***)

2. Set the optimal wobble width (***wbsw***) and the number of wobble steps (***wbst***) for the chosen channel

3. Set the broad-band channel on broad-band probes, to the configured nucleus. The first time after plugging in the PIC System connector, the auto configuration can take several minutes

4. Start a special wobble process to get the best resolution. The wobble curve may look unfamiliar

5. Open a window showing the various controls to operate the matching and tuning rods (see next chapter: ***atmm*** graphical user interface)

6. Stop the wobble process

7. Restart the process at step 4, if another channel was selected

8. Restore the old value for ***wbsw*** and ***wbst***

9. Terminate the ***atmm*** command with a specific status (description in chapter: Command Status)

The command ***atmm*** will open the control below.

Figure 3.1. ***atmm*** *control window*
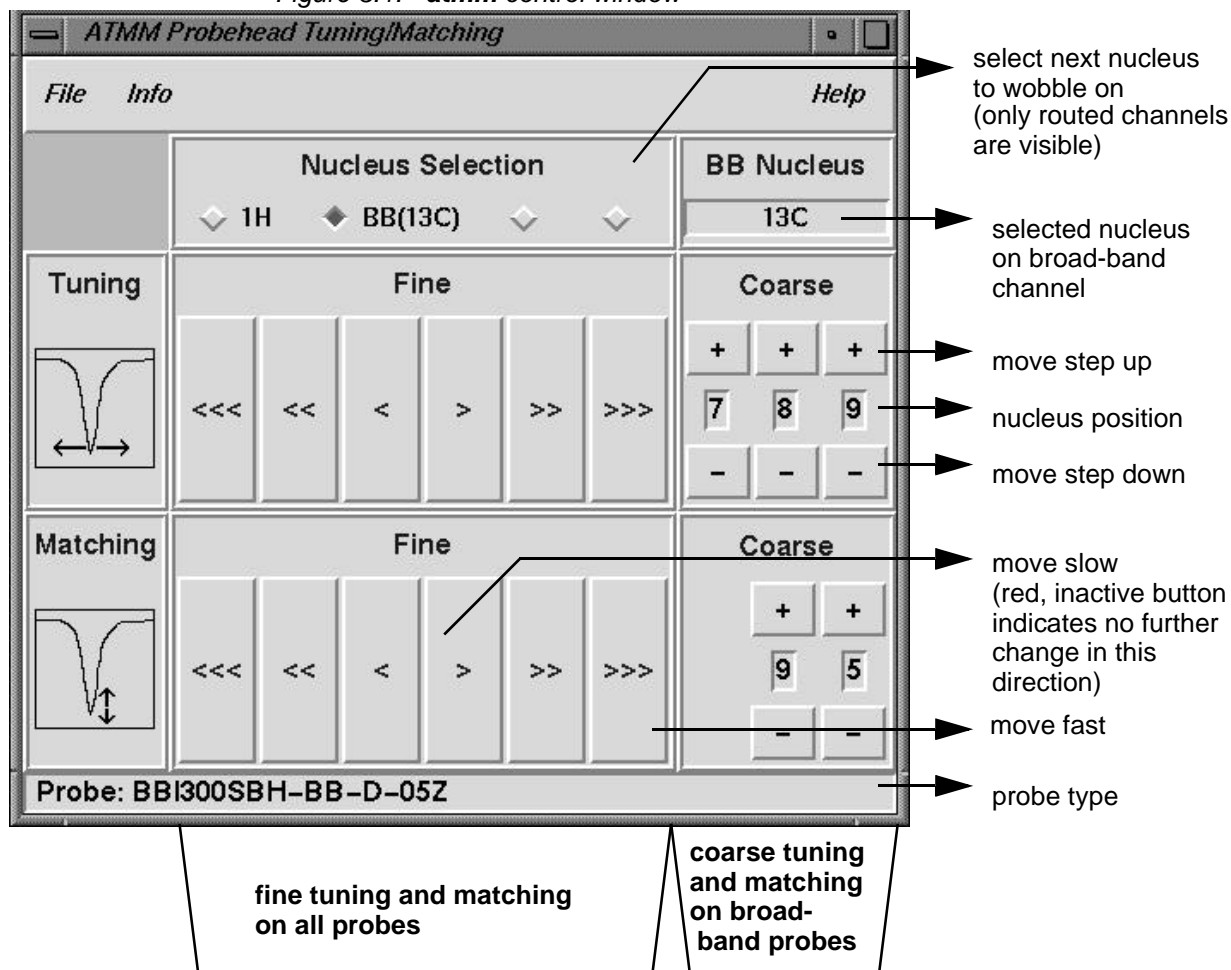
Menu structure

- ***File -> Quit***
  Close the window and terminate ***atmm***

- ***Info -> show broad-band nuclei***
  Opens the window which shows all known nuclei of a broad-band probe.
  (Negative nuclei positions are not set up now)

- ***Help -> About***
  Shows version of the user interface

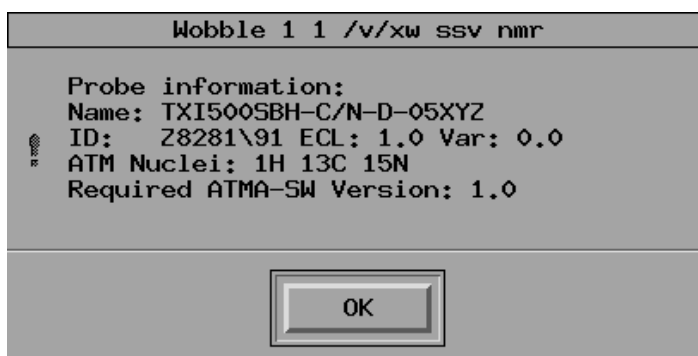| nuclei	freq	tune	match
31P	161.975	-799	99
87Rb	130.928	-798	98
13C	100.613	789	95
17O	54.245	-775	85
15N	40.545	-751	77
14N	28.904	-588	65
97Mo	26.618	-567	62

Software

Options for atma and atmm *3.2*

The table shows the available options for the commands **atma** and **atmm.**

Table 3.1.

Option	*atma*	*atmm*	Description
low	X	X	wobbles with all routed nuclei starting at the lowest frequency. This is also the default option
high	X	X	wobbles with all routed nuclei starting at the highest frequency
f1 - f8	X	X	wobbles the specified channels in the given order; example, f1 f3 f2 f1
ext50	X	X	takes the reference with a external 50Ohm terminator, instead using the internal 50Ohm reference. If the wobble process takes a long time to optimize, the reference may drift away
exact	X		gets the best optimization but can take a long time to complete
coarse	X		is faster to complete but will perform a less accurate optimization
noWin	X		shows no message window if **atma** couldn't find the optimum. Useful for scripts
version	X	X	shows the actual ATMA software version. No optimization will be done
probeInfo	X	X	shows information of the connected probehead. No optimization will be done
bbInfo	X	X	shows information about the broad-band nuclei. Nuclei without brackets can be used automatically. Nuclei in brackets do not yet have a verified nuclei position. Use the **atmm** to verify a nucleus. No optimization will be done
selectNuc	X	X	on broad-band probes, sets the broad-band channel to the configured nucleus and terminates the **atma** command. No optimization will be done
manWbsw		X	use the actual wobble width (**wbsw**) and the number of wobble steps (**wbst**) for the wobble process
? or wrong option	X	X	shows all available options for **atmm** and **atma.** No optimization will be done

- *atma* or *atma low*
  will automatically tune and match all observable routed channel starting at the lowest frequency

- *atma f2 coarse*
  atma f1 exact
  optimize tuning and matching for f1 (e.g.1H) very accurate and for f2 (e.g. 13C) fast

- *atma* selectNuc
  sets the broad-band channel to the requested and terminates the *atma* command. No optimization will be done

- *atma f1 f3 f1 noWin*
  will automatically tune and match the channel f1, f3 and again f1. If it get an error no message window will be shown

- *atmm f1 manWbsw*
  starts the wobble process on channel f1 using the actual wobble width (*wbsw*) and the number of wobble steps (*wbst*)

- *atma version*
  shows the version of the installed ATM software

- *atma probeInfo*
  shows the message window below

```
        Wobble 1 1 /v/xw ssv nmr

   Probe information:
   Name: TXI500SBH-C/N-D-05XYZ
   ID:   Z8281\91 ECL: 1.0 Var: 0.0
   ATM Nuclei: 1H 13C 15N
   Required ATMA-SW Version: 1.0



                 OK
```

Verify a new nucleus on the broad-band channel *3.3*

To set up the broad-band channel for a new nucleus the following steps must be done:

1. Check with the command **atmm bbInfo** if the nucleus can be used with the probe. The range of the broad-band channel is shown e.g. "31P-109Ag"

2. Connect the broad-band channel to a HPPR module which can wobble the requested nucleus, e.g. 2H can't be wobbled on some modules

3. Configure the nucleus with the **edasp** command (start with a low frequency nucleus, because they are easier to set up)

4. Start the command **atmm** to verify the new nucleus. This must be done once for every new nucleus (Note: this is also true for the factory predefined nuclei which are shown in brackets in the bbInfo window)
   The wobble width (**wbsw**) will be set very large. So the dip should be visible.

5. First use the tune coarse buttons (+ and -) to set the dip in the middle of the window, then use the match coarse button to get a good matching
   If no dip is visible set the wobble width manually. Exit the **atmm** command (don't save the position) and set the wobble width with **wbsw**. Now restart the **atmm** command with **atmm manWbsw**

6. Use the fine buttons (<, <<, <<<, >, >>, >>>) to get an optimized dip.
   If the button color is red, the dip can't move further in this direction. Set up the coarse position again (last step)

7. To check the position of the coarse buttons do one step up and down. The best position should now be between the two

8. Close the **atmm** window and save the new position

9. **atmm bbInfo** should now show the new nucleus. All nuclei without brackets can be used automatically

Command Status *3.4*

The **atma** and **atmm** commands return a status when they terminate. The status can take the following values:

- 0   Command executed successfully

- -1   Command not successful; resonance dip not found

- 3   Communication failed (PIC system)

- 6   System procedure error (wobble not possible)

Installing ATM Patch *3.5*

To install a new ATM Patch do the following steps

1. Verify with the command ***atmm version*** if the installed ATM Version is older then the latest available version

2. Get the latest version from the Bruker ftp-server.
    Example shows the version 2.0 for sgi
    ftp://ftp.bruker.ch/pub/NMR/download/atm/xwinnmr2.6/sgi/ atm2.0xwin2.6sgi.tar.Z

3. Copy the file to a empty directory

4. Uncompress the file with ***uncompress atm2.0xwin2.6sgi.tar.Z***

5. Unpack it with ***tar xvf atm2.0xwin2.6sgi.tar***

6. Become a superuser (requires the superuser password) ***su***

7. Start the installation program ***perl AtmaInst***

!   ***Note: In future new ATM versions are part of the xwinnmr and/or it's patches***

Troubleshooting *3.6*

If ***atmm*** or ***atma*** generate an error, check the following points

*   Is the cable on the probe and HPPR plugged in

*   Is the HF-cable attached to the right nucleus on the probe

*   Is the corresponding nucleus observable (HPPR module)

*   Can the selected channel be wobbled with the standard ***wobb*** command

*   Try to move the matching and tuning with the ***atmm*** command.

*   If the dip couldn't be optimized with ***atma***, try a second time

*   On broad-band probes if the requested nucleus couldn't be set, remove the PIC System connector on the probe and then re-connect it

Problem Description *3.6.5*

This issues has been reported to our development staff to be addressed in a future release.

*   WARNING: Error in preamp HPPR-1,
    error number=21, error code=Already error
    ->This warning does not affect ***atma*** or ***atmm***

Software