

Software Manual

Version 2.1



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Please make use of the report form at the end of the manual for comments, error reports, and suggestions.

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Chapter 1 Introduction

1.1 What is NMR-CHECK?

NMR-CHECK is an easy-to-use interface which offers features to test the basic functionality of Bruker NMR spectrometers. The major hardware components of Avance Spectrometers can be checked with just a few mouse clicks. This can be done either on-site, i.e., tests are started directly by the operator, or remotely by Bruker service personnel connected to the instrument over networks.

In addition to the check of individual components, a test of the entire spectrometer is available via Internet or ISDN. After establishing such a network connection, Bruker specialists can easily work at the operating systems level of the UNIX workstation. Hence, the spectrometer operator does not have to type in complicated UNIX commands that were told to him over the phone.

When a high-speed communication line is available, preferably via ISDN, NMR-CHECK offers a remote control function. This means that the entire spectrometer can be simultaneously driven by the local operator and a distant Bruker partner somewhere in the world. During this session both conferees use the same, wellknown XWIN-NMR interface.

1.2 Hardware/software requirements

Computer and Operating System:

- Silicon Graphics (SGI): CPU R4000, R4400, R4600, R5000. Operating System IRIX 5.3, 6.2, 6.3, or 6.5.
- *Spectrometer:* Avance or ARX/AMX2/ASX (for hardware tests only useful when equipped with HPPR or BSMS)

Software:

XWIN-NMR 1.3 or newer must have been installed prior to NMR-CHECK 2.1.

Release Medium:

NMR-CHECK 2.1 is delivered on the NMR-Suite CD containing XWIN-NMR 2.6.

Network access (optional but strongly recommended):

- *Internet:* Local routing of Bruker's IP addresses (class B: 149.236.) from the SGI workstation to the Internet via a gateway must be accomplished. The class-C subnet 149.236.99, however, must be routed to the console computer CCU via the second Ethernet port as usual.
- *ISDN:* Basic rate interface (two B channels) S_0 , D-channel protocol E-DSS1 (Euro ISDN) or 1TR6 (occasionally used in Germany) required. All services (telephony, fax, data transmission) have to be activated.

In addition, an ISDN telephone can be connected to the S_0 bus. When used, however, the maximum rate of data transfer is limited to 64 kbit/s (one B channel). You should avoid connecting any additional ISDN device.

ISDN cable: RJ-45 to RJ-45, pins 3 to 6 directly connected, up to 150 m long as measured from the Network Termination NT. Shielded (STP) or unshielded (UTP) twisted-pair cables can be used as well. Part numbers: 83024 (2 m), 83025 (5 m), 83026 (10 m).

Indirect ISDN access via an ISDN gateway is possible. Such a gateway must use the Password Authentication Protocol PAP. A permanent PAP access name and PAP password have to be allocated. Dynamic assignment of IP addresses is permitted.

SGI Indy workstations come with an ISDN controller built-in. O2 workstations require an external device, which must be connected to **serial port #1**. The following devices are currently supported:

- Elsa MicroLink ISDN/TL pro (ISDN terminal adapter; only for O2 workstations; Bruker part number: O001164)
- Elsa MicroLink ISDN/TL V.34 (ISDN terminal adapter/modem combination; must be connected to an S₀ interface; primarily for Bruker Service Centers; ISDN functionality only available on O2 workstations; Bruker part number: O001163)
- *Telephone network:* Conventional analog telephone interface. Supported external devices:
 - Elsa MicroLink 33.6TQV / 56k (high-speed modems; can be used with Indy and O2 workstations; Bruker part number: O001162)
 - U.S. Robotics 33.6 or 56K modems (can be used with Indy and O2 workstations)

1.3 Network security

NMR-CHECK is primarily designed to operate with computer networks, though it can also be used on isolated spectrometer workstations. To assure highest network security, the SGI computer should be connected to an ISDN interface. The most prominent security features implemented in NMR-CHECK include:

- NMR-CHECK can be launched by authorized personnel only. The password of the *NMR superuser* has to be entered. This password can be freely defined by the system administrator.
- NMR-CHECK prints a detailed warning if there is any account in the system that is not protected by a password (user account) or not locked (special account).
- NMR-CHECK supports shadow passwords.
- NMR-CHECK supports the Network Information Service (NIS).
- Remote access by Bruker is performed via a temporary *service account*. This account is automatically created when NMR-CHECK is started up. Its password and permissions have to be defined at the same time by the operator. The service account is automatically removed from the system when NMR-CHECK is terminated. This means that not even Bruker has access to the instrument when NMR-CHECK is not running.
- ISDN/modem access is a two-step process. Before logging into the system in the background via the service account, the ISDN call has to be established. This task is controlled by the *Password Authentication Protocol (PAP)*. The

necessary account for this purpose has to be created with NMR-CHECK and is not usable for any other system access.

• NMR-CHECK automatically logs the date, time, duration, and identification of any incoming and outgoing ISDN/modem call. Failures are also registered.

1.4 Version

This manual applies to NMR-CHECK version 2.1. NMR-CHECK contains this manual as on-line documentation accessible from the *Help* menu.

New feature added in release 2.1:

• Support of the modem 'Elsa MicroLink 56k'. -

The very successful 'Elsa MicroLink 33.6TQV' is getting out of stock. The successor model 'MicroLink 56k' complies with NMR-CHECK's specifications and is therefore recognized by NMR-CHECK version 2.1.

Note that 56K modems require a special digital device at the other end of the connection in order to provide faster data transfer (downstream) than 33.6K models. Don't expect to get any advantage over 33.6K modems during remote sessions with Bruker, because the major data flow is upstream, i.e., from the spectrometer workstation to Bruker's support computer during XWIN-NMR sharing.

If you want to know more about the 56K modem technology, visit the following Web sites:

<u>www.k56flex.com</u> (read the K56flex FAQ) <u>www.3com.com</u> (search for a white paper about the V.90 technology).

1.5 Support

Software support for NMR-CHECK is available from your local Bruker office or via e-mail from the following address:

<u>Michael.Hansen@bruker.de</u>

The Bruker FTP servers <u>*ftp.bruker.de*</u> and <u>*ftp.bruker.com*</u> provide additional information such as known bugs and their workarounds in the directories

/pub/nmr/NMRCHECK/ and /pub/nmr/mirror.bruker.de/NMRCHECK resp.

1.6 Installation of NMR-CHECK

NMR-CHECK can be separately selected as an installation item from the NMR-Suite installation dialog window SWIM. NMR-CHECK 2.1 can only work if XWIN-NMR 1.3 or newer as well as the ISDN Execution Environment (*isdn_eoe*), the Point-to-Point Protocol Software (*eoe2.sw.ppp* @ IRIX 5.3, *eoe.sw.ppp* @ IRIX 6.x), and the UUCP Utilities (*eoe2.sw.uucp* @ IRIX 5.3, *eoe.sw.uucp* @ IRIX 6.x) have been installed prior to NMR-CHECK. When using ISDN under IRIX 5.3, the installation of patches 363 and 531 is strongly recommended. Those patches are available from /*CDROM/unix/patches5.3*/.

1.7 Starting up NMR-CHECK

1.7.1 Operator restriction

NMR-CHECK can be started by anyone who has a login account on the SGI workstation. Click on *Find/Applications* inside the SGI Toolchest, and double click on NMR-CHECK's icon, which is shown in <u>Figure 1.1</u>. If the main window of NMR-CHECK does not pop up, open a console window by clicking on *System/Utilities/ Start New Console* (IRIX 6.3) or *System/Start New Console* (IRIX 6.2, 5.3), and try again. Alternatively you can start NMR-CHECK by typing



Figure 1.1 NMR-CHECK's desktop icon

nmrcheck

from a UNIX shell, no matter what directory you are in. You will be prompted to enter the *NMR superuser* password (cf. section 1.3). Ask your system administrator if you do not know this password.

1.7.2 Create a temporary service account

After the NMR superuser password has been typed in, a menu as shown in Figure 1.2 pops up.

NMR-Check 1.0
Define password for temporary service account: *******
Permission: full 💻
OK Exit

Figure 1.2 Definition of temporary service access

Type in a password of your choice with at least four alphanumeric characters. Characters in excess of eight are redundant as usual. *Permission: full* means that the service account will be equivalent to the root account. Thus, the entire file system can be inspected and corrected during an on-line session. *Permission: restricted* creates a service account which has the limited rights of a regular user. The service account is used for NMR-CHECK's diagnosis and UNIX support features. No password of any existing account has to be revealed, and no extra account has to be created by the system administrator in order to enable remote access. Clicking on *OK* causes the automatic generation of the service account. NMR-CHECK is now ready to use.

Keep in mind that the service account will be automatically removed from the system when NMR-CHECK is terminated (cf. section 1.3). If the account already exists at start-up time for some reason, you have to confirm the password update.

1.8 Using the mouse or the keyboard

Within NMR-CHECK, you can use the mouse or the keyboard to select items and execute commands, and to position the text cursor.

- In order to execute a function represented by a button or a menu item, either click on it using the left mouse button, or hit the *Enter* key once it is selected.
- In order to select the next or previous button in a window for execution with *Enter*, use the *Tab* or *Shift* +*Tab* keys.
- In order to select the next or previous menu item or list box item, use the *Down Arrow* or *Up Arrow* keys, or the left mouse button.
- In order to move the text cursor within text entry fields, use the *Left Arrow* or *Right Arrow* keys, or the left mouse button.
- Hitting the Enter key while editing a text field executes the Save function.
- In order to close a window, click on the right-most button (*Cancel* or *Quit*) or press the *Esc* key. The click-away function (double-click on the upper left corner of the window) is available only for login windows.
- The passwords for ISDN access (*Setup/Hosts Configuration/Modify/ISDN/ Password:*) and on-line service (*Setup/Hosts Configuration/Modify/Service/ Password:*) can be made visible by double-clicking with the left mouse button inside the entry field, or by selecting the field and pressing the *Print Screen* key.
- Computer names in list boxes can be chosen by double-clicking with the left mouse button.
- In addition to moving the scroll bar, browsing through list boxes can be performed by keeping the middle mouse button pressed inside the list box and moving the mouse appropriately. Alternatively, the *Page Up/Page Down* keys can be used when the list box has been selected with the *Tab* key.

1.9 Appearance of the mouse cursor

Outside entry fields, the mouse cursor appears as an *arrow*. When NMR-CHECK is working, the mouse cursor changes to a *watch*. During this time NMR-CHECK does not accept any user interaction. Be patient! Some of the diagnosis procedures take minutes until completion. Therefore, you will be informed about the approximate

duration of every single test. If you think that NMR-CHECK has crashed because it does not seem to be active anymore, wait a little longer. Terminate the UNIX processes belonging to NMR-CHECK only if you are positive that NMR-CHECK has crashed! In such a case, try to use NMR-CHECK's Emergency Exit, i.e., double-click the button in the upper left corner of NMR-CHECK's main window. If that does not help, terminate NMR-CHECK on the UNIX level. Note: The emergency exit function is deactivated during e-mail processing.

Warning: If you terminate NMR-CHECK on the UNIX level while an ISDN connection is open, this line might remain open (producing telephone charges)! In such a case, start NMR-CHECK again and stop it orderly with the *Exit* function.

1.10 Tear-off menus

All menus except *File* and *View* can be torn off by clicking on the dashed line at the top of the menu. You can move a tear-off menu to a place on the screen where it is always accessible. It will even stay open when NMR-CHECK's main window is being iconified. This feature is especially useful for the *Multidisplay* and *Diagnosis* menus.

Chapter 2 Getting started

2.1 General

This chapter is a compact guide to NMR-CHECK. For details, please refer to the full description of each function.

2.2 How to set up NMR-CHECK after installation

Fill out the form *Setup/General Profile*. Put in your data on the left-hand side and those of your contact at the Bruker service department on the right. Skip the rest of this section if you want to get on-line service via Internet, or if you just like to run diagnosis procedures yourself.

If your spectrometer workstation can be reached via ISDN/modem do the following:

• If you want to get on-line service from Germany and you are using an Indy workstation, fill in 7219511060 as Bruker's ISDN number in the *Setup/General Profile* form. If your service center is in Switzerland enter 18065820. Ask for alternative numbers if you operate an O2 computer. These numbers must be preceded by the code for long-distance calls to or in Germany and Switzerland, respectively. Don't forget any leading digit(s) required by the local telephone

network to make external calls. The Bruker ISDN lines are used for computer connections only. Don't dial these numbers with a telephone – no human being will answer.

- Execute *Setup/Hosts Configuration/Add*, enter "service" for example, fill in the same ISDN number as before, set *IPAddress* to "149.236.12.10" (Germany) or "150.205.48.51" (Switzerland), ask your Bruker contact for an *Access Name* and a *Password*, choose *Speed: High*, and set *Sleep if idle*? to *No*. You don't have to fill out the *Service* page.
- If you want to share XWIN-NMR with your Bruker contact, this person will normally do on-line service from his own computer, named "mike", for example. Therefore, you have to add host "mike" to the list of Remote Computers. You can leave the ISDN/modem parameters empty. Switch to the *Service* page, ask the Bruker person for "mike"'s IP address, set *Connect via* to *ISDN Card* (Indy)/*ISDN/TL*... (O2), and set *ISDN Host* to "service". Leave the *Password* field blank (you don't need a service password for XWIN-NMR sharing).
- Give Bruker the ability to call you. Execute *Setup/ISDN Access Restriction* and add "bruker", for example. Fill in a password of your choice, enter an optional annotation ("Bruker ISDN account", for example), and click on *Save*. Now, "bruker" should show up in the restriction list. Inform your Bruker contact about this ISDN account name and password by phone, fax or e-mail.
- Plug in the ISDN cable and execute *Setup/PPP Daemon*. If the PPP daemon is running, the *Start* button is deactivated and the active device and protocol types are shown. Click on *Restart*. If the daemon is not running, choose the correct protocol type (ask your ISDN provider) and click on *Start*.
- Now, you are hooked up for ISDN on-line service.
- Perform the same tasks if your computer is connected to an ordinary telephone interface via a high-speed modem. Choose the appropriate value from the device list and ignore the *Speed* and *Sleep* settings. The Bruker ISDN numbers can be used for modem links as well.

2.3 How to get on-line service

- If you can be reached via Internet, make sure the network parameters of your spectrometer workstation are properly configured (ask your network administrator).
- Stop any acquisition.

- Call your Bruker contact, start NMR-CHECK, type in the NMR superuser password (ask your system administrator), enter a Service Password of your choice, and tell the Bruker person that password.
- Open the *Setup/General Profile* form and read the IP address of your workstation (lower left corner). Fill in the *Service Contract Number*.
- If you can be reached via ISDN and it is the first time you use on-line service, tell your Bruker partner your ISDN number, the ISDN Access Name and the ISDN Password. Make sure the PPP daemon is running.
- If *you* have to open the ISDN line to Bruker, terminate XWIN-NMR. Open a sharing session to host "mike" (see previous section) with *Multidisplay/Share XWIN-NMR*. Iconify the sharing window as long as you don't perform XWIN-NMR sharing. Your Bruker partner will then use the ISDN line to open a spectrometer connection.
- Explain your problem and lean back. You won't see any result of a test sequence that has been started by remote service on your screen. Nevertheless, on-line service can only be performed as long as NMR-Check is running on your spectrometer.
- Terminate NMR-CHECK with *File/Exit* when the on-line session is over.

2.4 How to run diagnosis procedures yourself

- Double click on *Connect/Spectrometer/Local instrument*. Choose the component you want to test from the *Diagnosis* menu. Mark the test(s) to be performed and click on *Start*. The *Expert* page provides more advanced tests. The *Launch Tool* button is designed for Bruker service engineers don't perform any action with this interface unless you know exactly what you are doing.
- All diagnosis output is automatically logged and accessible over a period of eight days via *View/Test Results* and *View/Tools Log*.
- If an on-line service of your spectrometer is impossible for technical reasons, you can send the diagnosis results to your Bruker contact by e-mail or fax. Just choose the appropriate day via *File/Test Results/Send by Email* or *File/Test Results/Print as Fax*. The default e-mail address can be defined in *Setup/General Profile*. Fax printers can be easily set up with <u>cfpp</u> in XWIN-NMR.

Chapter 3 The *File* Menu

3.1 General

The *File* menu (<u>Figure 3.1</u>) provides functions for sending diagnosis results to Bruker via fax or e-mail. This main menu also lets you terminate NMR-CHECK.

Test Results	
Tools Log	
System Configuration	⊳
XWIN-NMR Location	
Upload	
Exit	

Print as Fax Send by Email Delete Today's

Figure 3.1 File's main menu and first submenu

3.2 Test Results/Tools Log

For an explanation of the difference between *Test Results* and *Tools Log* <u>see "Test Results/Tools Log" on page 50</u>.

3.2.1 Print as Fax

Clicking on *Print as Fax* creates a submenu showing the past eight days during which diagnosis results were obtained. Before you select a day for printing, view its contents with *View/Test Results* or *View/Tools Log*. Then, make sure you filled out the *Setup/General Profile* form (see "General Profile" on page 29). If you did not set up any printer yet, run cfpp in XWIN-NMR first. Now, click on the desired day. This will open an interface as shown in Figure 3.2.

NMR-Check 1.0	
PRINTER FOR FAX CREATION	
hpcljm hpdj660c kyf5000 laserjet	Δ
Print Cancel	7

Figure 3.2 Interface for fax creation

Select a printer and click on *Print*. As a result, you will get a fax-ready printout with cover sheet and numbered pages. Add comments by hand on the lower half of the cover sheet if you like.

3.2.2 Send by Email

Alternatively to printing and faxing diagnosis results to Bruker, you can send the same information via electronic mail. For this to work, the spectrometer workstation needs access to the Internet, i.e., to an Internet gateway in your local network.

If the workstation has not yet been set up for e-mail transmission proceed as follows:

- Become superuser and edit the file */etc/sendmail.cf.* After lots of comments, there is a section called "Parameters which MUST be defined". Replace the BAR.FOO.COM entries by the values of your local network. Ask your network administrator if you are not sure what to fill in.
- Run the UNIX commands

/etc/init.d/mail stop /etc/init.d/mail start

in order to restart the sendmail daemon.

• Under IRIX 6.3 /etc/sendmail.cf is different. Leave it as it is and run /usr/etc/ configmail setup instead. Read the explanations carefully, and confirm the restart question if you made changes. List the current settings with /usr/etc/configmail list.

Preview what you are going to send by executing *View/Test Results* or *View/Tools Log*. Click on *Send by Email* and then on the desired day. Confirm the question whether the default e-mail address, which was defined with *Setup/General Profile*, has to be used. Click on *No* and enter any address you like in order to send the diagnosis results to someone else.

3.2.3 Delete Today's

With the function *Delete Today's* you can clear the lists of diagnosis results which were obtained today. This is particularly useful when lots of results have been recorded, but only very few are of importance to Bruker's service personnel. After (irreversibly) deleting the results, you have to repeat the meaningful diagnosis procedures. Then, send the output via fax or e-mail as described above.

3.3 System Configuration

With *System Configuration* you can print a listing of important configuration parameters of the local system for fax transmission or send that compilation via email. You can preview the entire listing by clicking on *System Configuration* in the *View* menu. The preceding paragraph gives details on printer and e-mail setup.

3.4 XWIN-NMR Location

As of XWIN-NMR's release 2.0, the installation directory of XWIN-NMR can be freely defined. Furthermore, several copies of XWIN-NMR can coexist on one computer. Since NMR-CHECK uses test programs delivered by XWIN-NMR, it has to know where XWIN-NMR is located. If you intend to utilize a copy of XWIN-NMR which cannot be found via your environment variable PATH, click on *XWIN-NMR Location* and select the directory containing XWIN-NMR's binary files. This is usually the subdirectory *prog/bin/* of the directory path you chose to install XWIN-NMR in (see Figure 3.3).

NMR-Check 1.0	
INSTALLATION DIRECTORY OF XWIN-NMR BINARIES	
 / u prog bin install.net scripts 	
OK Cancel	

Figure 3.3 Declaration of XWIN-NMR's installation directory

If you are running NMR-CHECK in combination with XWIN-NMR 1.3, the menu item *XWIN-NMR Location* is permanently deactivated, because XWIN-NMR's installation directory is fixed.

3.5 Upload

After a connection to a remote spectrometer has been established with *Connect/Spectrometer*, the *Upload* entry becomes activated. Select a single file or a directory for transmission and click on *Send* (see Figure 3.4). In case of a directory selection, every file in that directory and recursively all the files in subdirectories will be packed into an archive named *upload.tar*. Symbolic links will be resolved (and must be resolvable) prior to transmission. The transmitted file or *upload.tar* is stored in the directory */usr/people/service/ncup* on the remote computer. You can easily get there: click on *Connect/UNIX* and type *cd ncup*. If a directory has been selected for transmission, move the archive *upload.tar* to the final destination and unpack it (*mv upload.tar* <*directory*>; *cd* <*directory*>; *tar xvf upload.tar*). For that purpose, the source files are archived with relative path names.

Press the *Stop* button at any time you want in order to terminate a running file transfer. The file fragments which have been already sent, however, will remain on the target computer. Therefore, the existence of the transferred file in the target directory does not necessarily mean that the transmission was successful. If in doubt, compare the file sizes of the source and target files, or verify the file identity by comparing the checksums (*sum -r <filename>*).

Due to its upstream nature, the *Upload* function is primarily intended for Bruker personnel. A similar download feature, which could be used by the operator whose spectrometer is being serviced, has not been implemented for security reasons. Please use Bruker's FTP servers (ftp.bruker.com and ftp.bruker.de) for file downloads.

3.6 Exit

Exit terminates NMR-CHECK in an orderly manner. Always close the program with this function. If you think that NMR-CHECK has crashed because it does not seem to be active anymore – wait. Some of the diagnostic procedures take minutes until completion. Also, most features have a time-out built in. If you still think that NMR-CHECK has crashed, try to use NMR-CHECK's Emergency Exit, i.e., double-click the button in the upper left corner of NMR-CHECK's main window. If that does not help, terminate NMR-CHECK on the UNIX level. In such a case, it is strongly



Figure 3.4 User interface for file transfer

recommended to restart the program immediately and to terminate it with the *Exit* function in the *File* menu. Note: The emergency exit function is deactivated during e-mail processing.

Chapter 4 The *Setup* Menu

4.1 General

The *Setup* menu (Figure 4.1) allows for the generation of complete parameter sets to access remote computers for on-line service and to receive ISDN/modem calls. In addition, a spreadsheet is available for customer and Bruker service identification. Those data are needed for the off-line transmission of diagnosis results. Most parameters have only to be set once, before the first network connection is opened.

	Hosts Configuration			
	ISDN Access Restriction			
	General Profile			
	PPP Daemon			
	Sound:			
\diamond	off			
\diamond	calm			
\diamond	medium			
\diamond	loud			

Figure 4.1 The Setup menu

4.2 Hosts Configuration

Click on *Hosts Configuration* in order to configure the network parameters of remote computers. An interface as shown in <u>Figure 4.2</u> will be opened.

NMR-Check 1.0			
	REMOTE C	OMPUTERS	
mbul mike mim			
moos present			
seri serimod service strike			
tango Add	Modify	Delete	Quit

Figure 4.2 Management of remote computers

Add:

Creates a new data set. The computer name must consist of one to seven alphanumeric characters. It does not need to be identical to the nodename by which the remote system is known to communications networks. The name, however, must not be the same as an existing *ISDN account* (see "ISDN Access Restriction" on page 25).

There are two pages with parameters: ISDN / Modem (Figure 4.3) and Service (Figure 4.4). Fill out the ISDN / Modem page when the remote computer has to be connected over a dial-in line. Ignore this page for Internet connectivity.

• *Phone #*: Fill in the complete phone number of the ISDN or telephone interface which the remote computer is connected to. Omit any non-numerical characters like brackets, parentheses, and dashes.

- NMR-Check 2.0			
SETTINGS FOR "PRESENT"			
♦ ISDN / Modem	💠 Service		
Phone #:	0613130976		
IP Address:	172.18.54.13		
Access Name:	bruker		
Password:	******		
Speed:	🔷 Medium		
	🔶 High (ISDN only)		
Sleep if idle?	🔶 Yes (ISDN only)		
	♦ No		
After:	60 Seconds		
Annotation:	Gifts Inc., DSX		
Save	Cancel		

Figure 4.3 Setup of ISDN parameters

- *IP Address*: The address of the target system can be easily obtained by executing *Setup/General Profile* on that computer (Figure 4.7). Please enter the address in dot notation as shown in Figure 4.3. Leave this field empty for connections to *ISDN gateways* which assign IP addresses dynamically!
- *Access Name*: This name is used for ISDN/modem access verification on the remote computer. Therefore, it has to be included in the access list (Figure 4.5) of the system which receives the call.

- Password: Password of the Access Name as defined on the remote system.
- *Speed: Medium* means that one B channel is used for the connection, resulting in a maximum transmission speed of 64 kbits/s. This is sufficient for on-line diagnosis and UNIX support. The second B channel can be used for a simultaneous telephone conversation over an ISDN telephone connected to the same ISDN interface.

High means that both B channels are permanently bundled for fastest data transmission. This setting is strongly recommended for XWIN-NMR sharing (see <u>"Share Xwin-nmr"</u> on page 38).

For modem links, the speed setting is irrelevant. The transfer rate over a telephone link is automatically set to 33600 bits/s in either direction. In order to achieve the maximum transmission speeds when using external devices, the baud rate of serial port #1 must be set to a much higher value. This is automatically done by NMR-CHECK depending on the device type and the computer model. (Note: External ISDN terminal adapters cannot be used with Indy workstations, because the baud rate of their serial ports is limited to 38400 bits/s.)

• *Sleep if idle?*: If set to *Yes*, the ISDN line will be temporarily closed when no data transfer occurred during the period of time as set in the line *After: Seconds*. This interval has to be in the range between 30 and 300 seconds. The connection is automatically re-established (after about 10 seconds) when any data flow to or from the remote sytem appears. This setting is primarily useful for UNIX support. It has no effect during XWIN-NMR sharing.

For modem links, the sleep mode setting is ignored. It would take about 30 seconds to reactivate the line, which is unreasonable.

- *After*: See above.
- Annotation: Enter an optional, descriptive text of unlimited length here. The annotation is displayed in brackets after the host name in the Setup/ Hosts Configuration, Connect/Spectrometer, and Multidisplay/Share XWIN-NMR interfaces.

Fill out the *Service* page (Figure 4.4) for remote diagnosis, no matter what network type is used. Ignore this page when configuring an ISDN gateway. Customers use the *Service* page to define the Bruker computer on which the display for XWIN-NMR sharing has to appear.

- *IP Address*: See above.
- *Password*: Enter the password which the remote operator defined at the start-up of NMR-CHECK (see "Create a temporary service account" on page 8). For cus-

tomers only: (1) Fill in any password you like when this computer can be directly accessed for XWIN-NMR sharing. (2) Leave this field blank when the computer is reached via a Bruker ISDN gateway (see *ISDN Host* below).

- Connect via: Choose the network and device type to be used for the remote connection. This setting shows up as the default in the Connect/Spectrometer (Figure 5.2) and Multidisplay/Share XWIN-NMR interfaces (Figure 6.2) and can still be changed in there. ISDN Card refers to the built-in ISDN interface of Indy workstations. ISDN/TL must be selected on O2 workstations for establishing ISDN links. Modem 33.6/56k is the choice when using the high-speed modem from Elsa. Modem TL V.34 means that the universal adapter MicroLink ISDN/TL V.34 should be used in analog mode, i.e., to connect with a remote modem. Click on Modem Sportster if a high-speed modem from U.S. Robotics is connected to your computer.
- *ISDN Host*: When setting *Connect via* to any value but *Internet*, *ISDN Host* is automatically set to the name of the computer which is being configured (for remote service or XWIN-NMR sharing). This means that this target computer is *directly* connected to an ISDN/modem interface. Set *ISDN Host* to the name of an already defined ISDN gateway when the target computer is connected to that gateway via Ethernet, i.e. *indirectly* connected to the ISDN/telephone network.
- Annotation: See above.

Modify:

Opens the parameter pages of the selected remote computer. See under *Add:* for a description of the parameters.

Delete:

Deletes the entire parameter set of the selected remote computer and removes the computer name from the list.

4.3 ISDN Access Restriction

Click on *ISDN Access Restriction* in order to define access names and passwords to be sent by other computers which try to open an ISDN/modem line to your workstation. An interface as shown in <u>Figure 4.5</u> will be opened.

NMR-Check 2.0			
SETTINGS FOR "PRESENT"			
🔷 ISDN / Modem	♦ Service		
IP Address:	172.18.54.13		
Password:	*****		
Connect via:	ISDN/TL =		
ISDN Host:	present -		
Annotation:	Gifts Inc., DSX		
Save	Cancel		

Figure 4.4 Setup of service parameters

Warning: Your computer accepts incoming ISDN/modem calls when the *Activated* part of the access list is empty. Then, the knowledge of any existing login account and its password is sufficient to open the dial-in line and to log in to the system. This is a severe security leak. Therefore, you will be immediately requested to add an entry or warned not to remove the last entry. In other words, always define at least one entry in this list if your computer is connected to an ISDN/modem interface while the PPP daemon (see "PPP Daemon" on page 29) is running.

- NMR-Check 2.0			
USERS ALLOWED	TO CONNECT TO THIS H	HOST VIA ISDN OR MODEM	
Activated		Deactivated	
ettli [Hansen & Co, Ettlingen] secura [Security account]	× ×	bam [Bruker Analytik, Rheinstette bii [Bruker Instruments, Billeric bvs [Suttner KG, Wiesbaden] mpip [MPI-Polymerforschung, Mainz] sadis [Bruker France, Wissembourg] sag [Bruker AG, Faellanden] swm [Yellowstone Inc., Brookfield wstr [Universitaet Rahlstedt]	
Add	Modify	Delete Quit	

Figure 4.5 Management of ISDN access accounts

Add:

Creates a new ISDN access account, or activates an existing account from the *Deactivated* list.

Steps to create a new account:

- 1. After typing in a non-existing name, an interface as shown in Figure 4.6 pops up.
- **2.** Type in a password of your choice (four characters or more). Inform the remote party about the password.
- 3. Fill in a short description of the remote party into the field Annotation.
- 4. Click on *Save*. The new account will be added to the access list.

Modify:

Select a user from the access list and click on *Modify* in order to change the account's password or annotation. The password field will always be empty when the interface pops up. If you leave that field empty and click on *Save*, the password

NMR-Check 1.0			
NEW ISDN USER			
Name:	remedy		
Password:	*****		
Annotation:	Bruker Service		
Save	Cancel		

Figure 4.6 Configuration of a new ISDN access account

will not be changed (useful if you want to change the annotation only).

Delete:

Select a user from the access list and click on *Delete* in order to remove that ISDN access account *permanently* from the system.

>>:

Select a user from the *Activated* list and click on >> in order to revoke ISDN access for that account *temporarily*. This account can be easily reactivated with the << button.

<<:

Select a user from the *Deactivated* list and click on << in order to re-enable ISDN access for that account.

Note: ISDN access accounts created with the *Add* button cannot be used for any other system access (see "Network security" on page 5). Accounts that have been tampered with will not be shown in the access list and cannot be used for ISDN/ modem access.

4.4 General Profile

Click on *General Profile* and fill in all data (see Figure 4.7) in order to identify yourself when sending diagnosis results by e-mail or fax to Bruker. ISDN numbers can be left blank if you do not have ISDN access. With the *Reset* button you can empty all entry fields. Network features like sending diagnosis results and XWIN-NMR sharing require a valid *Service Contract Number*. Call your Bruker Service Center if you do not have one. In addition, the *Service Contract Number* is displayed on the monitor of Bruker's service computer while a remote spectrometer connection is being established.

The *Domain Name* and *IP Address* of the local workstation are listed for informational purposes. If a remote connection to a spectrometer has been opened via an ISDN gateway which assigns IP addresses dynamically, the current address is displayed on Bruker's profile form. This temporary address has to be made known to the customer in order to share XWIN-NMR successfully.

4.5 PPP Daemon

Click on *PPP Daemon* for managing the PPP daemon. This daemon has to run in order to make and receive ISDN/modem calls. When the daemon is *stopped*, the setup interface will appear as shown in Figure 4.8, i.e., *Restart* and *Stop* buttons are deactivated. Select a *Communication Device* that corresponds to the telecommunication hardware available at your computer (for details about the button values see <u>"Connect via" on page 25</u> and <u>"Hardware/software requirements" on page 4</u>). Then, you have to select the local D-channel protocol to be used by clicking on the *ISDN Protocol Type* button. That button becomes deactivated, however, if one of the dedicated high-speed modems (connected to a conventional telephone interface) is chosen. Ask your telephone company if you are uncertain what protocol type is used. *External Device Name, Serial Number*, and *Firmware Version* are automatically detected everytime the PPP daemon interface is started if a supported communication device is connected (takes a few seconds). Note: An external ISDN adapter or modem **must be connected to serial port #1**!

When the PPP daemon is *running*, the *Start* button is deactivated (see Figure 4.9). *Communication Device* displays the device type/operation mode for which the PPP daemon has been activated. The *ISDN Protocol Type* button shows the type of protocol that is running if an ISDN device is in use. In other words, the two topmost

NMR-Check 1.0			1.		
GENERAL PROFILE					
	Local Data		BRUKER		
Company/Institution:	MPI f. Polymerforschung				
Address:	Postfach 3148 D-55021 Mainz, Germany				
Contact:	Dr. P. Carbonat	Contact:	Dr. M. Hansen		
Phone (Lab):	(06131) 123-456	Phone:	(07243) 504-449		
Fax:	(06131) 123-789	Fax:	(07243) 504-480		
ISDN:	(06131) 13579	ISDN:	(07243) 997755		
Email:	pc@mpip.de	Email:	mih@bruker.de		
Spectrometer Type:	DSX 800				
System Order #:	HH987654				
Service Contract #:	0815/97				
Indy's Name:	spock.software.bruker.de				
IP Address:	149.236.14.32				
Sau	re F	Reset	Cancel		

Figure 4.7 General profile form

buttons reflect the current daemon configuration. You can click on *Restart* to stop and start the daemon again. This is often very useful when the activation of a telecommunication line has failed. Select other device or protocol values and hit the *Restart* button if the daemon is misconfigured. The *Stop* button must be used to terminate the PPP daemon. This is the software equivalent to unplugging the ISDN or modem cable. Note that it is impossible to restart or stop the PPP daemon as long as an ISDN/modem connection is active. For security reasons, the termination of NMR-CHECK automatically stops the PPP daemon. Additionally, unplug the ISDN or modem cable if you want to prevent anyone from calling your computer.

NMR-Check 1.1				
MANAGEMENT OF PPP DAEMON				
Communication Device:	ISDN Card			
ISDN Protocol Type:	Euro ISDN 💻			
External Device Name:	(no device detected)			
Serial Number:				
Firmware Version:				
Start Restart	Stop			

Figure 4.8 Interface to start up the PPP daemon

4.6 Sound

Select a sound level to customize the dialing and error noises. NMR-CHECK always starts with *calm* as the default value. Note: On O2 workstations, the lowest possible, still audible sound level *calm* is quite loud.

- NMR-Check 1.1				
MANAGEMENT OF PPP DAEMON				
Communication Device:	ISDN/TL			
ISDN Protocol Type:	Nat. ISDN (Germany) —			
External Device Name:	MicroLink ISDN/TLpro Rel. K			
Serial Number:	0409.019.161 K 00005			
Firmware Version:	Ver. 2.20K vom 27.01.97			
Start	Stop Cancel			

Figure 4.9 Interface to restart or terminate a running PPP daemon

Chapter 5 The *Connect* Menu

5.1 General

The *Connect* menu (Figure 5.1) is used by Bruker personnel to open network connections to spectrometer workstations. When such a connection has been successfully established, the *Diagnosis* menu becomes active and tests can be performed. In addition, the *UNIX* function can be used for support at the operating system level, and files can be transferred with *Upload* in the *File* menu.

You have to initialize your spectrometer with the *Connect* menu before being able to run tests locally. In this case, the *UNIX* function is not needed, and therefore the button remains deactivated.

Spectrometer	
UNIX	

Figure 5.1 The Connect menu

5.2 Spectrometer

Click on *Spectrometer* in order to initialize a diagnosis session either to a remote or to the local NMR spectrometer. An interface as shown in <u>Figure 5.2</u> will be opened.

NMR-Check 1.1	.1
SPECTROMETER TO CONNECT FOR DIAGNOSIS	
Local instrument berghau berlin cisco	
egger eole guest heinz jens	
	II Y I
Connect via: ISDN Card = ISDN Host: egger =	4
Connect Disconnect Cancel	

Figure 5.2 Interface to control network connections

The list of computer names is similar to the one configured with *Setup/Hosts Con-figuration* (cf. Figure 4.2). Hosts which have been set up with a missing service password (cf. Figure 4.4) will not be listed (this password is essential for a remote diagnosis session)!

The list entry *Local instrument* is always present and does not depend on the setups performed with *Hosts Configuration*. If it is absent, the file */etc/hosts* is corrupt.

Connect via: and ISDN Host:

When selecting a remote spectrometer, the default values as defined with *Setup/ Hosts Configuration/Service* will be set. See <u>"Connect via" on page 25</u> and <u>"Hard-ware/software requirements" on page 4</u> for more details. If a telecommunication link has been already established (via XWIN-NMR sharing or from a remote computer), the *Connect via* button is locked. In that case, NMR-CHECK automatically detects the parameters of the existing link and uses that line if possible.

Connect:

Opens the network connection to the selected remote spectrometer, or initializes the local instrument. When the connection has been successfully activated, a green box as shown in Figure 5.3 appears at the lower right corner of the screen. This box can be moved to any place by clicking on it with the left mouse button and dragging the mouse while keeping the button pressed. If the *Sleep if idle* function has been set and the inactivity timer has elapsed, the box turns red and "active" becomes "sleeping". This behavior will be reversed if the connection could be re-established.



Figure 5.3 Connection indicator

In the case of a remote connection, a bar graph display will be automatically opened. This is identical to clicking on *View/Network Traffic*. For details see "Network Traffic" on page 50.

If the connection is running via ISDN/modem, a *PPP Status* window is launched. On Indy workstations, an additional *ISDN Status* window will be generated. The status display(s) can be opened by clicking on *View/On-line Statistics* as well. For details see "On-line Statistics" on page 52.

Note that the acquisition will be automatically locked on the selected spectrometer. This is necessary to avoid conflicts between diagnosis procedures and an acquisition on the spectrometer.

Disconnect:

Closes the current spectrometer connection. If the line is sleeping, NMR-CHECK tries to reactivate it in order to remove the acquisition lock from the remote machine.

5.3 UNIX

The menu entry *UNIX* becomes active when a connection to a remote spectrometer has been successfully opened. Click on it to get a login window. You will be automatically logged in using the temporary service account. The ability to perform efficient UNIX support depends on the type of permission which the remote operator defined at start-up (see "Create a temporary service account" on page 8).

If you are planning to launch XWIN-NMR from the remote login window, you will not be able to start any acquisition. In order to reactivate acquisition for the rest of the on-line session, click on *Yes* after the question "Do you want to perform acquisition on spectrometer '...'?" appears. Keep in mind that this may interfere with diagnosis procedures.

Any number of login windows can be opened. Close each window with the clickaway box (double click on the button in the upper left corner of the window frame), by typing *exit*, or by pressing Ctrl-D when the mouse cursor is in that window.

Chapter 6 The *Multidisplay* Menu

6.1 General

The *Multidisplay* menu (Figure 6.1) is used by customers to open a special conference mode, which is called *application sharing*. During such a conference, an application program running on the customer's computer, like XWIN-NMR, is shared with a specialist at Bruker. This means that an identical copy of the application's display appears on the monitor of the conferee (WYSIWIS – What You See Is What I See). Either party has full access to all functions of the shared program.

Share XWIN-NMR	
Share Whiteboard	
Restore Colors	
Stop Sharing	

Figure 6.1 The Multidisplay menu

Of course, only one user can drive the application at a time. Therefore, some additional conversation is necessary. This can be done over the phone or via *Share Whiteboard*. The person who has been chosen to be passive just releases the mouse. Then, he will see two mouse cursors: his own being steady, and an inverted one from the active person.

The only way for customers to open a telecommunication line to Bruker is to start an XWIN-NMR sharing session. If that line is used by Bruker to perform diagnosis procedures, all sharing windows should be iconified to avoid unnecessary data transfer.

Note that it is impossible to share an application that has been started in the normal, unshared fashion. Therefore, you cannot share a copy of XWIN-NMR which has been launched outside NMR-CHECK.

Application sharing is based on the program "XMX 2.1a-pl5". Portions of this software are copyright Brown University, Providence, RI, 1991-1996. Brown University makes no representations about the suitability of this software for any purpose. The portions owned by Brown University are provided 'as is' without express or implied warranty from Brown University.

6.2 Share XWIN-NMR

In order to share XWIN-NMR, you have to define the Bruker computer where the conference partner is located. If this computer is not directly connected to the ISDN, you have to configure the ISDN gateway first (see <u>"Hosts Configuration"</u> on page 22 and <u>"How to set up</u> Nmr-check after installation" on page 11). Note there must be a workstation at Bruker which is not protected by a firewall, in order to share XWIN-NMR with Bruker via Internet.

Warning: Assuming that XWIN-NMR sharing is technically possible over the Internet, make sure the connection is stable and fast. Otherwise, responses to a single mouse click can take one minute or more to appear at the remote site.

Clicking on *Share XWIN-NMR* will open an interface as shown in <u>Figure 6.2</u>. Before you start a sharing session do the following:

- 1. Start XWIN-NMR outside NMR-CHECK as the same user you started NMR-CHECK.
- **2.** Resize the width of the total XWIN-NMR window to about two thirds of the screen width.
- **3.** Type <u>setres</u>, set *2D-Mode* to "Contour", set *Editor* to "xedit", click on *Apply*, and close the interface.

NMR-Ch	eck 1.1				1
	COMPUTER	то зна	RE XWIN-NM	IR WITH	
heinz jens mbu1 mike					
mim moos present seri service strike					Y
${\triangleleft}$					
Share via:	ISDN Card	-	ISDN Host:	service	-
	Share		ļ	Cancel	

Figure 6.2 Share XWIN-NMR interface

- 4. Exit XWIN-NMR.
- **5.** For O2 workstations: Terminate all other applications which make extensive use of colors, like XWIN-NMR started by other users, Netscape, and so forth.

Select the computer where your Bruker partner is located. The values for *Share via* and *ISDN Host* will be set to the defaults as defined with *Setup/Hosts Configuration/Service*. See <u>"Connect via" on page 25</u> and <u>"Hardware/software require-</u> <u>ments" on page 4</u> for more details. If a telecommunication link has been already established (via *Connect/Spectrometer* or from a remote computer), the *Share via* button is locked. In that case, NMR-CHECK automatically detects the parameters of the existing link and uses that line if possible. Click on *Share*. Display tools for monitoring the transmitted data will be opened (see <u>"Network Traffic" on page 50</u> and <u>"On-line Statistics" on page 52</u> for details). Next, an empty window pops up in which XWIN-NMR is automatically started. On O2 workstations, expect a delay of about 10 seconds until the XWIN-NMR interface appears on the screen. This is the *sharing window* where the conference will take place. A window of the same size and content is launched at the remote computer.

At first sight, the sharing window looks like an ordinary XWIN-NMR interface. You can identify it easily, however, by its window title ("... Shared XWIN-NMR" at the local computer, "xmx" on the remote screen). In general, the shared copy of XWIN-NMR behaves like the normal one. There are a few exceptions:

- The XWIN-NMR display is not resizable.
- New interfaces like <u>search</u> and <u>setres</u> cannot be moved.
- Special processing like phasing, scaling and movement of the displayed data, which is performed by pressing a mouse button and dragging the mouse while keeping the button pressed, behaves differently. Normally, the degree of processing action depends on the mouse speed. In sharing mode, the action only depends on the distance the mouse has been moved. Even when the mouse has been stopped, while keeping the button pressed, the processing action continues! This makes the mouse more sensitive.

If you want to terminate such a processing action, you must, therefore, release the mouse button.

• When you share XWIN-NMR 2.5 or newer, the following commands do not work: <u>BarcodeSxInfo</u>, <u>cfbest</u>, <u>cflims</u>, <u>clbest</u>, <u>config</u>, <u>cpan</u>, <u>gradshim</u>, <u>iconnmr</u>, <u>masrmon</u>, <u>protocol</u>, <u>smail</u>, <u>temon</u>, <u>uxresources/setres</u>. These commands run with Tcl/Tk interpreters, which are based on Tk 4.1 or newer. As of release 4.0, Tk is incompatible with NMR-CHECK's sharing software.

When you start one of those functions, it will immediately fail without a message, i.e., nothing happens. However, an associated process *xwish2* or *xwish3* remains running, which can be terminated with XWIN-NMR's <u>kill</u> command.

Commence the XWIN-NMR conference by demonstrating your problem. Then, release the mouse and let your Bruker partner take over the activity. He will try to track down the problem, for instance, by inspecting acquisition and processing parameters, pulse programs, and so forth. If necessary, he will start an acquisition, and you can observe its progress on-line. In order to share XWIN-NMR successfully, obey the following rules:

- Use ISDN in high-speed mode.
- Be patient! During an XWIN-NMR conference, large amounts of data have to be transferred over the line. Every little motion of the mouse in the 1D display window causes a screen refresh. Therefore, do not unnecessarily move your

mouse across the sharing window. Note that your local sharing copy of XWIN-NMR reacts nearly as fast as usual, but the remote copy is delayed by the ISDN transfer speed.

- Do not click several buttons too quickly after each other. Wait until the completion of a complex action has been confirmed over the phone or on the shared whiteboard by the remote person, before you execute another function. Also, watch the "Thruput" column in the middle of the *ISDN Status* window (Indy workstation): The remote screen has been updated when the throughput goes down to zero. When using an O2 computer, keep an eye on the columns "Obytes" and "Ibytes" of the "ppp0" line shown by the *PPP Status* display at the local and remote host, respectively.
- Avoid "special processing" as described above, where a short mouse movement causes a flood of data.
- *Never* close additional windows, like the ones created with <u>setres</u>, <u>search</u>, or <u>xwinplot</u>, by using their exit function! This may terminate the entire sharing session. Type <u>kill</u> instead and click on the application to be terminated.
- Turn off the sharing of mouse movements by clicking on *Telepointer* (see below) if the conference is held via a conventional modem link.

If the convenient way of switching the input activity by just moving the mouse becomes a problem, the input permission of one conferee can be temporarily revoked. This can be achieved by enlarging the sharing window to the right. An interface as shown in Figure 6.3 appears.

E File	Select	Prefs	Telepoin	ter
Add Drop	spostr			
Floor Seat View				
Grab				

Figure 6.3 Interface for configuring the sharing permissions

The two icons symbolize the conferees, identified by the name of the computer they use (abbreviated to the first three letters). Select the conference partner and click on *View*. The icon will loose its hat and hammer. As a result, that person cannot drive XWIN-NMR anymore. Nevertheless, he can still see what the conference partner is performing in the sharing window. The active conferee can reactivate the passive one by clicking on *Floor. Seat* also deactivates the selected person, but it only removes the icon's hammer. This is different from the *View* mode in that the passive conferee can click on his icon, which then rises an arm. With this, he can signal his partner that he wishes to become active again.

If one conferee is in *View* mode, the performance can be improved by clicking on *Telepointer*. As a result, movements of the mouse cursor will no longer be displayed in the sharing window of the conference partner. This eliminates undesirable screen refreshes. This is especially useful when sharing XWIN-NMR over a high-speed modem line. It is not recommended to click on *Telepointer* if both conferees are in *Floor* mode. This can easily lead to the false and confusing conclusion that a currently active partner is idle.

The other buttons of the interface in <u>Figure 6.3</u> do not perform any useful function. Therefore, do not use them.

Terminate an XWIN-NMR sharing session with the menu entry *Stop Sharing* (see below). Typing <u>exit</u> in XWIN-NMR will certainly terminate XWIN-NMR, but the (empty) sharing window will remain running.

6.3 Share Whiteboard

The *Share Whiteboard* button becomes active when an XWIN-NMR sharing session has been successfully opened (see previous section). Click on it to share a whiteboard (notepad) with your Bruker partner. An extra sharing window as shown in <u>Figure 6.4</u> will pop up. This window is independent of the XWIN-NMR sharing window.

The whiteboard is intended for written conversation. Perform the following steps:

- 1. Click on *Size* in the bottom line with the *right* mouse button until "Font size 20" is displayed in the status line above.
- **2.** Click on *T* in the tool box.



Figure 6.4 Shared whiteboard

3. Click on the notepad and enter text. Terminate each line by pressing *Enter*. Do not move the mouse before you press *Enter*, because the text you just typed in may be cleared by a screen refresh.

Characters of the current line can be deleted by hitting the *Backspace* key. The cursor keys have no effect. In order to delete a line, click on *skull and crossbones* in the tool box, move the mouse cursor over that line, and click on it with the left mouse button.

Be careful when creating drawings, because they might congest the data line.

Terminate the shared whiteboard with the menu entry Stop Sharing (see below).

6.4 Restore Colors

If running XWIN-NMR on O2 workstations under IRIX 6.3, the data display is blacked out when the mouse cursor enters a certain class of applications (e.g., *View/Network Traffic* or */usr/sbin/clock*). This effect is cancelled when the mouse cursor travels back into the XWIN-NMR window. During XWIN-NMR sharing, the other parts of XWIN-NMR's display might change colors as well. This happens in particular if another "color-consuming" program (e.g., Netscape or XWIN-NMR started by a different user) is running at the same time. Click on *Restore Colors* in order to refresh the sharing display.

Hint: Stop all applications but NMR-CHECK prior to establishing XWIN-NMR sharing. Then, *Restore Colors* should not be needed.

6.5 Stop Sharing

Stop Sharing closes all sharing windows on either computer, and it terminates the conference. If the XWIN-NMR sharing window is closed while there is still significant data throughput on the line, the termination signal cannot reach the remote computer. This leaves a frozen sharing window on the remote screen, which can be easily removed with the click-away button.

Stop Sharing also terminates the ISDN/modem connection if it is not used by any other on-line activity of NMR-CHECK.

Chapter 7 The *Diagnosis* Menu

7.1 General

The *Diagnosis* menu (Figure 7.1) is used to check the major hardware components of remote spectrometers or of the local instrument. The menu entries become active after a spectrometer connection has been successfully opened with the *Connect/Spectrometer* interface (see "Spectrometer" on page 34).

CCU
TCU
FCU
RCU
GCU
ACB
RX22
BSMS
HPPR

Figure 7.1 The Diagnosis menu

Click on one of the component names to open a new interface, specialized for that part of the instrument. The interfaces for *CCU*, *ACB*, *HPPR*, *BSMS*, and *RX22* pop up immediately. The ones for *TCU*, *FCU*, *RCU*, and *GCU* will be created after a delay of about 15 seconds.

7.2 Handling of the diagnosis interfaces

The structure of all diagnosis interfaces is similar. <u>Figure 7.2</u> shows the BSMS interface as an example.

MMR-Check 1.0		
Measure helium level Activate keyboard Calibrate RCP pulses Sweep shims Calibrate spinning Check lock source Launch Tool	Select: All None Mode: ♦ Standard ♦ Expert	Bruker Smart Magnet Control System
Calibration of spinning (takes about 2 minutes ERROR: p109 from SLCB: Sample doesn't rotate - Check the sample. - Check cable and connector. - Check the console pressure (3-6 M - Check the pressure connector. <*><*><*> End of spinning calibration [Jaw	s) bar. typ.4 bar). n. 27, 11:55] <*><*>	
Measuring helium level (takes about 15 seconds Helium level [%]: 89 <*><*>> End of helium measurement [Jan.	s) 27. 11:56] <*><*> 	

Figure 7.2 Typical diagnosis interface

Test functions:

The box in the upper left part contains the available diagnosis procedures. Just click on the function names or the preceding check boxes for selection. You can combine any number of tests.

Launch Tool:

Launch Tool opens an extra interface, which requires special knowledge. It is intended for Bruker service personnel, in order to access rarely used test procedures and special hardware parameters. The best way of terminating the extra interface is to click on the same button as before, which is now labeled *Stop Tool*. After closing the diagnosis interface, the complete output is still accessible with *View/Tools Log* (see "Test Results/Tools Log" on page 50).

Open Console:

In the case of the *CCU* interface, *Open Console* replaces the *Launch Tool* button. Click on it to open a new window in which communication between the workstation and the CCU can be performed. This requires a special cable (delivered by Bruker; part number for Indy workstation: HZ04161; part number for O2 workstation: HZ10034) to be connected between the **serial port #2** of the workstation and the Console Port of the CCU board. Keep this cable connected all the time.

If the CCU is running, i.e., it was successfully booted, a CCU UNIX prompt appears in the console window. Otherwise, nothing will be displayed. Also, you will not get any error message from within this interface, because it is designed to monitor the basic output of the CCU board, no matter what it is. If the console window remains empty after pressing the red restart button of the board, check whether the cable is properly connected.

The best way of terminating the console window is to click on the same button as before, which is now labeled *Close Console*. After closing the diagnosis interface, the complete output is still accessible with *View/Tools Log* (see "Test Results/ Tools Log" on page 50).

Select All/None:

Simply selects all or no diagnosis function(s).

Mode Standard/Expert:

Switches between two diagnosis pages. *Standard* offers general and often used tests, *Expert* shows more specialized functions.

Listing of test results:

Every test prints its approximate duration immediately after start-up. Note that the running time may vary if errors occur. Subsequently, the test results will be listed.

The kind and amount of output strongly depends on the performed test function. Finally, the name of the test and the time of its completion are listed. You always have to wait until this final line appears before being able to perform another action.

Start:

Starts the selected diagnosis procedures. During tests which run about two minutes and longer, a progress bar is shown in the lower right corner of the listing area. This bar visualizes the degree of completion. Be patient – firmware downloads can take up to 25 minutes per board!

Halt:

If more than one test has been selected, *Halt* will terminate the sequence after the current test is over. You cannot interrupt a running test.

Reset:

Reset clears the listing area and deselects all test functions. The test results are still viewable with *View/Test Results* (see "Test Results/Tools Log" on page 50).

Cancel:

Cancel closes the interface. As long as the current spectrometer connection remains open, the current listing of test results will be redisplayed when the same diagnosis interface is opened again.

Chapter 8 The *View* Menu

8.1 General

The *View* menu (Figure 8.1) gives access to diagnosis results recorded in the past, it lists the current and past activity of the ISDN/modem interface, and shows general system parameters relevant for NMR experiments.

Test Results	⊳
Tools Log	⊳
Network Traffic	
Dial-up Connections	⊳
On-line Statistics	
System Configuration	
Intro	
Nothing	

Figure 8.1 The View menu

Listings are always shown in the display area of NMR-CHECK's main window. If some related action takes place while a particular listing is on the screen, that list

will not change automatically. You have to update the listing by clicking on the same function again. The on-line tools *Network Traffic* and *On-line Statistics*, however, are permanently updated. Clicking on these two functions has no effect when the corresponding window is fully visible. Otherwise, the tool display will be de-iconified or unobscured.

8.2 Test Results/Tools Log

Test Results allows you to review the entire output from diagnosis procedures that were started with this copy of NMR-CHECK. A submenu shows the past eight days during which test results have been produced. Click on the day you are interested in. Then, the complete listing of that day can be browsed. A header shows the creation date of each listing, which is identical to the time when the first test was started, and gives the identification of the local workstation. Each test result is preceded by a heading that shows the spectrometer on which the diagnosis procedure was performed. The local instrument is represented by the system name as stored in the file /*etc/sys_id*.

Tools Log does the same as *Test Results* but handles the logged output of *Launch Tool* and *Open Console* (see "Handling of the diagnosis interfaces" on page 46).

8.3 Network Traffic

Clicking on *Network Traffic* opens a bar graph display as shown in <u>Figure 8.2</u>. The number of bars can vary between two and four.



Figure 8.2 Network Traffic display

The bars labeled "NetTCP Act" and "NetIF [ec0]" are always present. "NetIF [ec1]" or "NetIF [ec2]" is shown when the O2 or Indy workstation, respectively, contains a second Ethernet controller, which is always the case on computers directly connected to and driving the NMR spectrometer. "NetIF [ppp0]" is displayed while a dial-up connection (via ISDN adapter or modem) is open.

The *upper number* at the end of each bar represents the value at full deflection. Therefore, each tick mark equals to a tenth of this value. This scaling is automatically recalibrated, for each bar independently, when the data throughput changes significantly. The *red value* in the middle is the maximum deflection. If this peak value has not been exceeded during the past ten seconds, it will be reset to the current value (peak-hold function). The *lower number* represents the average, calculated over a period of three seconds.

NetTCPAct measures the total data throughput for the Transmission Control Protocol (TCP) in kilobytes per second. *NetIF* [...] denotes the Network InterFace given in brackets. *ec0* is the name of the Ethernet port usually connected to a Local Area Network (LAN). The console computer CCU is normally connected to the Ethernet port *ec1* (O2 workstation) or *ec2* (Indy workstation). The ISDN port of the built-in card (Indy) and serial port #1 (connected to an ISDN adapter or modem) is called *ppp0* when in use. All interface traffic is measured in *packets* per second. Note that the packet size is variable and limited to about 1500 bytes for Ethernet and ISDN/telephone network.

8.4 Dial-up Connections

With *Dial-up Connections* you can list all ISDN and modem calls that came in or went out. Normally, two periods are available; one usually starts on the previous Sunday, the other one covers the week before. Outgoing calls are identified by the remote host name. Incoming calls show the ISDN access name (see "Setup of ISDN parameters" on page 23), which was transmitted by the remote system. The activation and deactivation of the telecommunication line as well as the duration is accurately listed. On Indy workstations, links which use the built-in ISDN interface are listed with a separate entry for each B channel. Mixed up entries and durations result from connection failures, where the switching order of B channels becomes unpredictable. Successful channel bundling (high-speed mode) is not software-detectable if an external ISDN adapter is used and, therefore, no distinction is made in the *Dial-up Connections* listing. High-speed ISDN links can be

identified by an orange "DCD" LED, however. That LED turns green for mediumspeed links (one B channel).

8.5 On-line Statistics

Clicking on *On-line Statistics* opens a status display as shown in Figure 8.3. Two "ppp0" lines appear if an attempt was made to open a telecommunication link (via ISDN or telephone network) since the last reboot of the workstation. An *asterisk* (*) behind "ppp0" indicates that the ISDN/modem interface is currently *not* in use. Watch the colums "Ibytes" and "Obytes" of the lower ppp0 line, as they monitor the number of incoming and outgoing bytes per second at the ISDN/modem interface, respectively. If an external ISDN adapter or modem is used, some information about the data flow can be also obtained from the LED's "TxD" (transmitted, i.e., outgoing data) and "RxD" (received data). The upper ppp0 line is not automatically updated on computers running under IRIX 5.3. If you are interested in the current content of that line, double-press the key *N* while the mouse is inside the PPP status window, or close the status display and open it again. On Indy worksta-

1: Interface Statistics Oct 6 18:17:57					D: Delta/second				
Name Mtu ec0 1500 ec1 1500 lo0 8304 ppp0 1500	Network 192,168 149,236 loopback (pt-to-p	.1 .99 < ot)	Address dummy ASP_ST2 localhost split						
Name ec0 ec1 lo0 ppp0	Ipkts 5 0 34	Ierrs 0 0 0 0	Ibytes 390 0 49776	Opkts 0 0 0 15	0enns 0 0 0 0	Obytes 0 0 600	Coll 0 0 0 0	q 0 0 0 0	trop 0 0 0
1:Interface	e 2 :Hb u	f 3:Str	reans 4:IP	5:ICHP	6:TCP	7:UDP 8:MCas	t DZF	N:no	ode

Figure 8.3 PPP status display

tions, an additional display pops up (see <u>Figure 8.4</u>). Each B channel of the built-in ISDN interface is monitored separately. The upper part shows the data throughput for outgoing and incoming traffic. All values are updated every second when an ISDN connection is open. Most important are the "Thruput" columns. They show

the effective transmission rate in kilobits per second, averaged over intervals of five seconds. Note that the values can exceed the theoretical limit of 64 due to compression.

ISDN	l connectio	on status	: Jan 2	9 10:27:40	1997				
	== Sent ==				== Received ==				
	Packets	Bytes	Dropped	Thruput	Packets	Bytes	Dropped	Thruput	
B1:	994	286640	0	64.0	772	13883	0	0.4	
B2:	295	194941	0	64.0 128 1	102 874	2006	0	0.4	
OCIN +	. 1200	401001	Ň	120.1	014	10000	Ň	0.1	
	Status		Phon	e Number	Rate				
B1:	Connected	ł	5044	79	64				
B2:	Connected	d	5044	79	64				
Line	e activity:	: *							
Q: 0	uit Z: Z	Zero cour	rts R: R	estore cou	nts L: Rec	lisplay			

Figure 8.4 ISDN status display

The lower part of the interface displays the connection status. Watch the "Rate" column. "64" means that the corresponding B channel is currently active, no matter what the throughput is. "0" indicates an unused channel. "Phone Number" displays the dialed number for *outgoing Euro ISDN calls* only. When the interface is closed and restarted while the line is still open, the telephone number will no longer be displayed. The phone number of incoming calls is never recognized. The "Status" column may show arbitrary information. Therefore, always watch the column "Rate". The ISDN status tool was written by Silicon Graphics. For that reason, we do not have any influence on those malfunctions.

The PPP and ISDN status displays can be closed by double clicking on the button in the upper left window corner, or by pressing q while the mouse is in the status display.

8.6 System Configuration

Click on *System Configuration* to get a listing of important configuration parameters of the local system. This includes general properties of the workstation as well as NMR-related characteristics.

8.7 Logo/Intro/Nothing

Logo displays the start-up logo. It will vanish if you click on it. *Intro* shows NMR-CHECK's greeting. *Nothing* clears the listing area.

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NMR-CHECK Comment Form

(Please mail to software support group. The address is printed on the second manual page.)

Name / Institution / Company:
Address:
Phone /Fax /E-mail:
Spectrometer / Computer:
Operating System / NMR-CHECK Version:
Comments / Error report / Suggestions (continue on extra sheet if required):