CryoPanel

- User Manual

Version 002

Innovation with Integrity

NMR

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Getting Started 1

What is CryoPanel? 1.1

CryoPanel is a graphical user interface (gui) for controlling a Bruker CryoProbe™ system. CryoPanel is equivalent in functionality to the CryoTool software, which to date, has been the standard tool for controlling and monitoring a CryoProbe™ system.

In contrast to CryoTool, CryoPanel is a fully integrated module within TopSpin. This integration allows additional capabilities, including the ability to stop an experiment when the cryoplatform goes into a ‘warm up‘ mode.

The CryoTool software is still necessary for DRX spectrometers and for systems that are equipped with the BSNL (Bruker‘s Smart Liquefier System) accessory.

Software Requirements 1.2

To use CryoPanel, Topspin 2.1 patch level 2 or later is required. TopSpin 2.1, in turn, needs to run on a PC with Windows XP Professional, Windows Vista, Linux WS3, or Linux WS4.

Installation of CryoPanel 1.3

CryoPanel is a module within TopSpin and, as such, the necessary software for CryoPanel is installed when TopSpin is installed for ‘Data Acquisition‘. In order to ‘activate‘ CryoPanel, though, some additional steps are required. Typically, these steps would be performed by a Bruker Engineer. For those customers wishing to install the software on their own, detailed instructions are included in Appendix A.1.

Version Information *1.4*

CryoPanel consists of two software components, the CCS (CryoControl Server) and the CryoPanel software. Information about the version of these software components can be found on the *Main Tab* of CryoPanel (see Figure 2.1).

Description of CryoPanel

2

General Notes 2.1

Once CryoPanel has been installed and the cryocontrol server started (see Appendix A.1), the program may be initiated by typing `cryopanel` on the command line of TopSpin. The CryoPanel layout consists of six separate sections, each of which is accessible by clicking on a Tab (see Figure 2.1). When CryoPanel is first opened, it exists as a window within TopSpin. CryoPanel may be detached from TopSpin by clicking on the detach icon ( ) in the upper left corner of each of the tab windows. Similarly, it may be reattached to TopSpin by clicking again on the same icon. Note that in either case, ***if TopSpin is closed then CryoPanel will also be closed.***

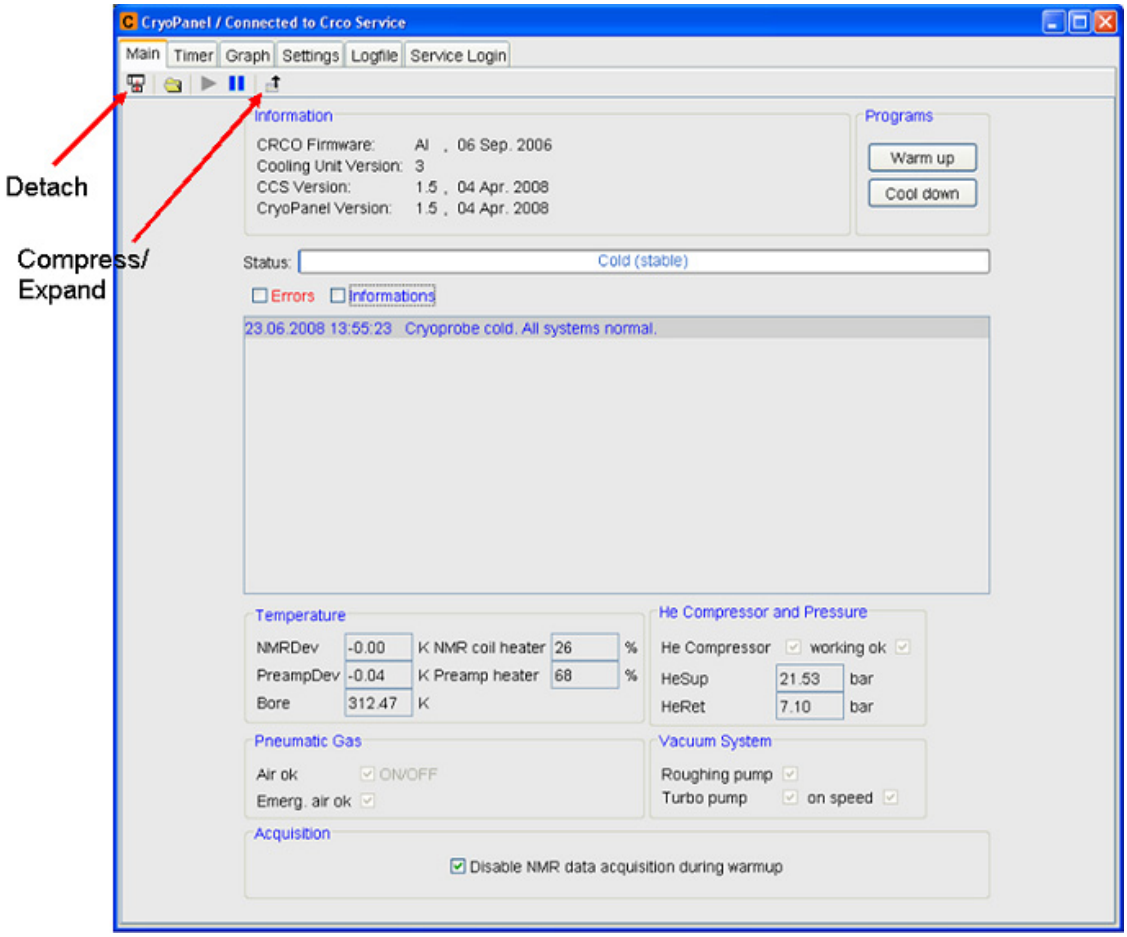

Figure 2.1. Main Tab Display of CryoPanel when it is first opened. By default, the initial display is in Expanded View.

The information displayed within the different tabs (especially the *Main* and *Graph Tabs*) will vary depending on the display mode. The display mode depends on two things:

- Compressed versus Expanded view - The *Main* and *Graph Tabs* have an icon in the upper right side that toggles between a compressed or an expanded view (or).

- User versus Service mode - If a service password is entered via the *Service Login tab* (see Section 2.7), additional information that is necessary for service purposes only, is displayed in some of the windows. Only the user-mode windows will be described in this manual.

A description of the different tabs is contained in the following sections.

Main Tab *2.2*

Main Tab, Expanded View *2.2.1*

The *Main Tab* Expanded View is the first view any user will see when opening CryoPanel (Figure 2.1). Most importantly, this window is where the user may issue the command to Cool Down or Warm Up a CryoProbe™. In addition, this view also shows version information and displays several status parameters. Brief descriptions of the various parameters are included below:

1. **Warm Up/Cool Down Buttons** - These are equivalent to the warm up/cool down buttons on the cooling unit. When selected, either a warm up or a cool down of the cryoplatform will be initiated. Please refer to the CryoProbe™ User Manual for more details.
2. **Information Section** - The information section lists several items which may be helpful for troubleshooting purposes. This includes the firmware (CRCO Firmware) version, the Cooling Unit Version, the cryocontrol server (CCS) Version, and the CryoPanel Version.
3. **Status Bar** - This horizontal bar attempts to graphically portray the progress of either a cool down or a warm up. When the system is cold and operating normally, the bar will display the message ‘Cold (stable)‘.
4. **Message Window** - This box in the center of the window displays messages from the cryoplatform. The messages may include instructions for the user (e.g., ‘Warm up started, remove sample now! (coldhead stops soon)‘), as well as error information for any problems encountered.
5. **NMRDev:** This is the deviation (in K) of the NMR coil temperature from its setpoint. In the cold state, this temperature deviation is close to zero. If the deviation is between 5 - 15k, the cryoplatform will indicate that the decoupling power is set too high and the COLD lamp on the cooling unit will start blinking. If this value exceeds 15K, an error which warns the user about an expected warm up will appear. Temperature deviations larger than 20k will initiate an automatic

warm up of the cryoplatform. *This is an important parameter which should be monitored whenever a new experiment is being set up - see the CryoProbe™ User Manual for more information!* NOTE: During a cool down, this parameter will be at a value of -1K until the system starts regulating the NMR coil temperature.

6. **PreampDev**: This is the deviation (in K) of the CryoProbe™ preamp from its setpoint. In the cold state, this value typically fluctuates a few tenths of a degree from the setpoint. Large deviations will lead to the issuing of information and error messages by the cryoplatform. An automatic warm up will be initiated if the deviation exceeds 14k. While this parameter is important, it is usually more helpful to monitor the Preamp heater parameter (see item 9 below). NOTE: During a cool down, this parameter will be at a value of -1K until the system starts regulating the preamp temperature.
7. **Bore**: This is the sample temperature of the CryoProbe™. This temperature is analogous to (but not quite the same as) the temperature indicated in the TopSpin edte window. If the Bore temperature is outside the given operating temperature range of the CryoProbe™ (consult the CryoProbe™ documentation for a specific range), it will force an automatic warm up of the cryoplatform. Be aware that it is the Bore temperature reading which determines whether the probe is outside its acceptable operating temperature range.
8. **NMR coil heater**: This is the value of the heater power being applied to regulate the temperature of the NMR coil. This value will vary depending on the cooling unit firmware version and it is normally around 20-25%. This value will typically fluctuate as it attempts to regulate the temperature of the NMR coil (such as during decoupling experiments).
9. **Preamp heater**: This is the value of the heater power being applied to regulate the temperature of the CryoProbe™ preamp. This value will vary depending on the cooling unit generation. Overtime, the preamp heater power will decrease from its optimum value of 80% for cooling units 1 - 3 and 140% for cooling unit 4. When this value falls below 10%, the WARM lamp on the cooling unit will start blinking and a full warm up/cool down cycle will soon need to be performed. *This is an important parameter to monitor over time as it indicates the performance of the overall system - see the CryoProbe™ User‘s Manual for more information!*
10. **Air ok**: This is an indicator of whether the main air pressure to the cryoplatform is within the acceptable range.
11. **Emerg. Air ok**: This is an indicator of whether the backup air pressure is within the acceptable range. Note that this parameter is ONLY relevant if the Sample Protection Device accessory is installed on the cryoplatform.
12. **He Compressor, working ok**: These boxes indicate whether the helium compressor is switched on and running.
13. **HeSup**: This is the helium supply pressure coming from the compressor. The absolute value of this pressure will depend on a variety of factors. More important than the absolute value is the stability of the trend of this parameter over time (see Figure 2.4).
14. **HeRet**: This is the helium return pressure going to the compressor. The absolute value of this pressure will depend on a variety of factors. More important than the absolute value is the stability of the trend of this parameter over time.
15. **Roughing pump**: This is an indicator of whether the mechanical roughing pump in the cryoplatform is switched on.

16. **Turbo pump**: This is an indicator of whether the turbomolecular pump in the cryoplatform is switched on.
17. **On Speed**: This is an indicator of whether the turbomolecular pump has reached an acceptable rotational speed.
18. **Disable NMR Data Acquisition during warm up** - This check box at the bottom of the window determines the behavior of TopSpin during a Warm Up. Generally this box should be left in its default setting (checked). When the box is checked, TopSpin will halt an experiment if the cryoplatform goes into a Warm Up mode.

Main Tab, Compressed View *2.2.2*

The user may toggle the expanded view in the *Main Tab* to a compressed view with the  and  icons (see Figure 2.1). The main difference with the compressed view is that it does NOT display the status parameters at the bottom of the screen.

Timer Tab *2.3*

The *Timer Tab* gives the user the ability to conveniently schedule cool downs or warm ups of the cryoplatform (Figure 2.2). Ideally, these processes could be scheduled overnight to minimize system downtime. The window is set up so that the user may schedule up to five different events (timers). To use the timer feature, the user would

1. Select any available timer from the ‘List of Timers‘ in the middle of the window
2. Select a date and enter a time at the bottom of the window
3. Select a process from the drop-down list (either ‘Cool_down‘ or ‘Warm_Up‘)
4. Select the Set/Replace Timer button

To make a change to an existing timer, the user would

1. Select the timer to be edited
2. Make the change(s) to the time, date, and/or process
3. Select the Set/Replace Timer button

Note that as soon as the Set/Replace Timer button is pressed, the timer is considered ‘active‘ and will be sorted chronologically according to its execution time. The display will change so that the *Timer Tab* of CryoPanel will contain a red square

(see Figure 2.3). This red square will remain until all of the timers have been completed, or until all of the timers are removed (with the Remove Timer button). An executed timer will automatically be deleted from the timer list.

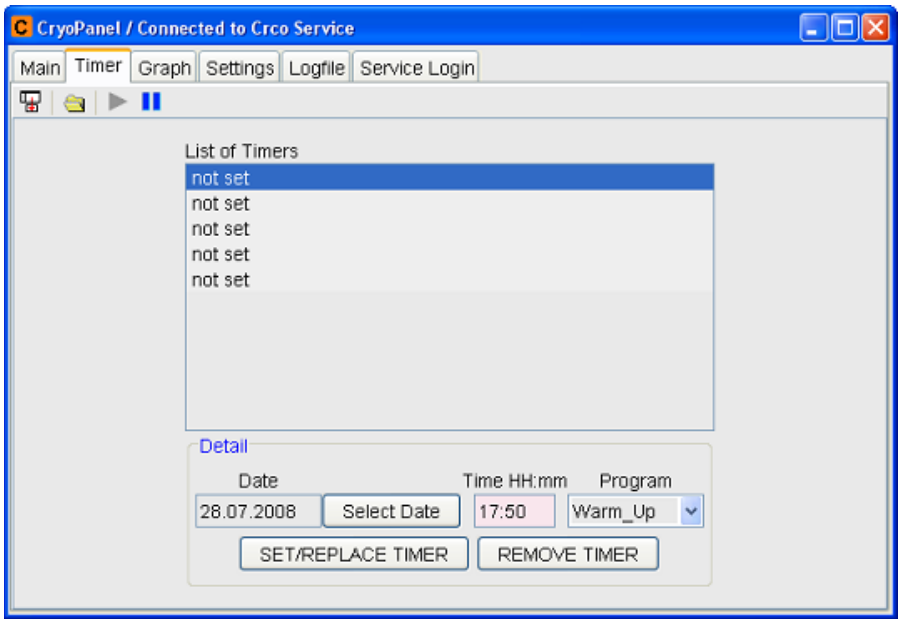

Figure 2.2. Default Timer Tab display, with no timers active.

Figure 2.3. Default Timer Tab display, with an 'active' timer. The red square on the Timer Tab indicates that a timer is active.

Graph Tab 2.4

In many cases, the status parameters for the cryoplatform at any given time are not as useful as are the actual trends in the parameters. The *Graph Tab* provides the user the ability to see many of these parameters plotted over time.

Graph Tab, Expanded View 2.4.1

Figure 2.4 shows the expanded view a user will see when first opening the *Graph Tab*. In this view, the user may view graphical information for all of the parameters which are listed in the *Main Tab* display (temperature deviations, heater power, bore temp, helium pressure) - see Section 2.2.1 for descriptions of these parameters. Left-clicking on the name of an individual parameter will toggle the graphical display of that parameter on or off.

Underneath each of the listed parameters, the user has the option to enter values to change the vertical scaling (/div) or offset. Using the icons at the top of the window, the user also has the option to change the time base, either by choosing the Zoom icons (, ,), choosing the preset 1 hour (1H), 1 day (1d), or 2 week (2w), or by choosing the left or right shift icons (,).

When adjusting the time base icons, the user must pay attention to the pause ( ) and resume ( ) icons. By design, one of these icons will always be greyed out to indicate whether the software is updating the readings. If the horizontal scaling is adjusted such that the present time is no longer visible on the display (e.g. when zooming into a past section of the display with mouse drag), the readings will stop updating - in that case, the resume icon must be selected to restart data acquisition.

Graph Tab, Compressed View 2.4.2

As with the *Main Tab*, the user may toggle the *GRAPH Tab* between a compressed and expanded view with the and icons. In the compressed view, the *Graph Tab* will NOT show the status parameters at the bottom of the window.

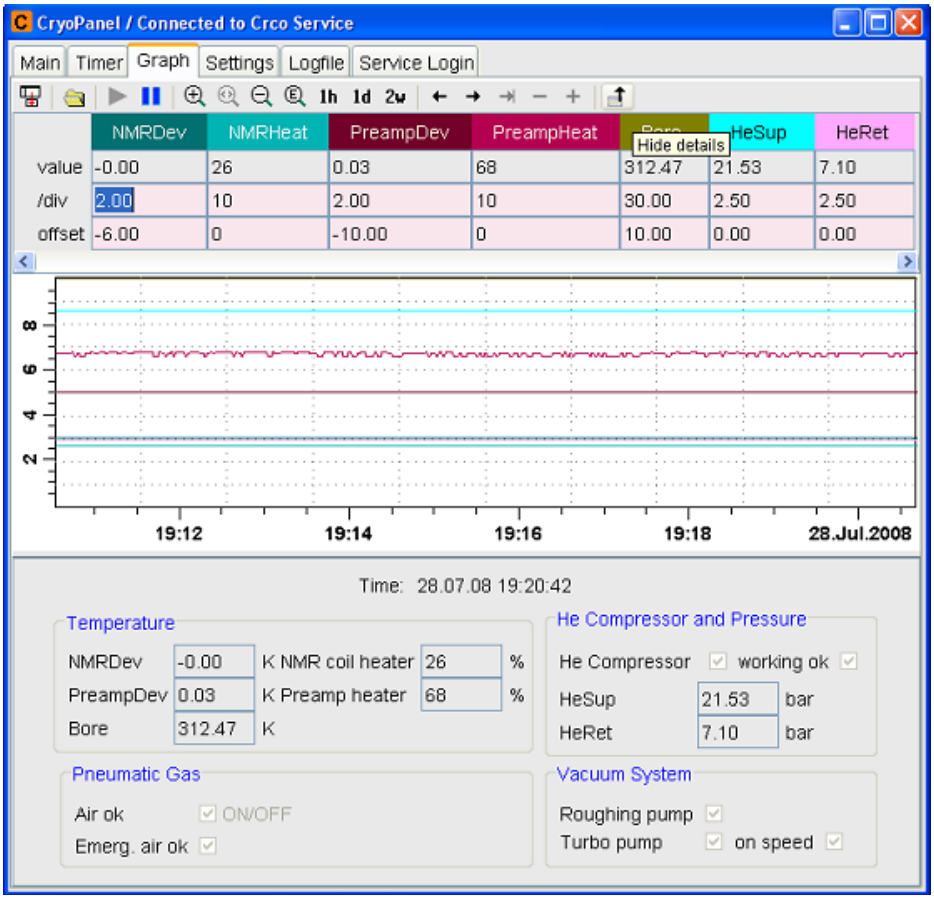

Figure 2.4. Graph Tab in User mode, expanded view.

Settings Tab *2.5*

The *Settings Tab* (Figure 2.5) gives the user the ability to change some configuration parameters for the cryoplatform. Descriptions of the options are as follows:

1. **Probe Type** - This setting allows the user to choose a probe profile before a cool down. The default is a standard 5/10mm probe.
2. **Cool Down Settings** - This setting allows the user to pull vacuum on the probe for a set period of time before starting a cool down. To activate this feature, the ‘Wait for user confirmation to proceed with cool down‘ check box must be selected and the time to wait (Timeout) in hours must be entered. When this option is selected AND a cool down is started *from the COOL DOWN button within CryoPanel*, the system will pull vacuum on the probe for the specified amount of time before proceeding with the initial flushes. A pop-up window will appear during this vacuum hold period where the user can give permission to proceed immediately (instead of waiting the prescribed amount of time).

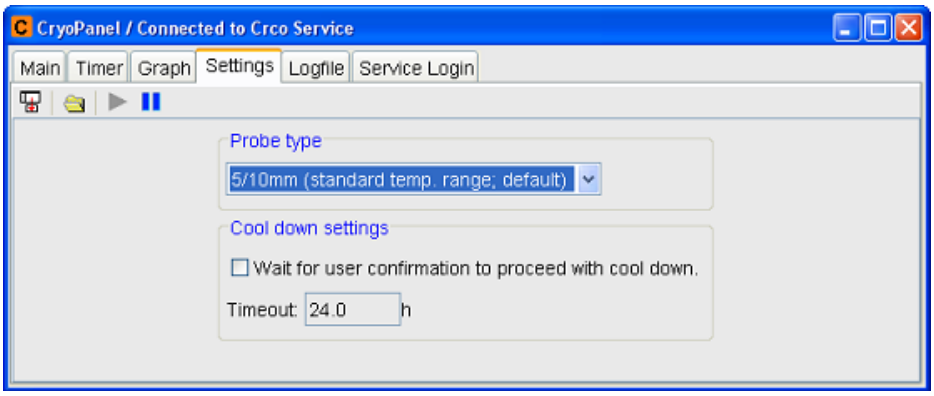

Figure 2.5. Settings Tab display in standard user mode.

Logfile Tab *2.6*

From the time that a Cool Down is initiated until the time that the platform is completely warmed up, CryoPanel (more specifically, the cryocontrol server) will keep logfiles containing all of the relevant temperature and pressure readings. This data logging occurs whether or not CryoPanel (or TopSpin) is running, as long as the PC is turned on and the cryocontrol service has been started (see Appendix A.1).

The *Logfile Tab* (Figure 2.6) is primarily used for saving the data logged by CryoPanel into a file which can be analyzed by a Bruker Engineer for diagnostic purposes.

The general procedure for saving logfiles is to

1) Select a file format (usually CryoTool)

2) Select a period of time

3) Click on the SAVE ( ) icon

4) Choose the file name/location to save the file

Once the SAVE icon is clicked, CryoPanel will save the data into a SINGLE logfile which can be emailed. More details about the steps in this procedure are given below.

1. **CryoTool versus CryoPanel format** - The choice of file format for saving logfiles is primarily related to the sampling time of the data. Files written in CryoTool format contain fewer sampling points, and hence are much smaller in size. In addition, CryoTool format files are saved in a compressed form with a *.zip extension, which leads to even smaller file sizes (as opposed to the *.bin extension of CryoPanel format files). In general, the user should ALWAYS choose the default CryoTool format for saving files, unless otherwise directed by a Bruker Engineer.

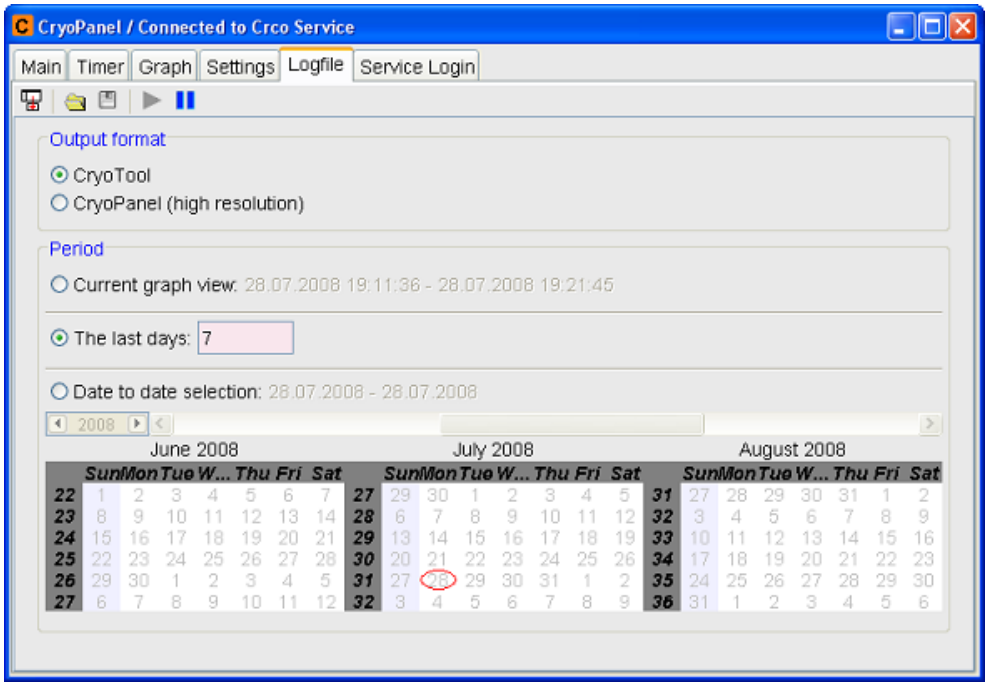

Figure 2.6. Logfile Tab. Unless otherwise instructed, the user should always choose the CryoTool format.

2. **Period** - The user has three options for selecting a range of data to save:

    a. The current graph view

    b. The last *n* days

    c. Date to Date selection

The user must select the button for the desired option, and choose the data range accordingly. For the most part, the data range selection is self-explanatory.

3. **Saving the Files** - After a format and a data range are selected, the user MUST click on the SAVE icon ( ) to actually store data. CryoPanel will then display a file browser suggesting a filename and a storage location. The user is free to change either the filename or the location, although the suggested values are recommended. A typical filename would be of the form

    YZxxxxxx_CPdateTOdate.ext

where *YZxxxxxx* is the Bruker ordering number of the NMR console and *ext* is the appropriate extension (*.zip for CryoTool format, or *.bin for CryoPanel format). Note that the YZ number will ONLY be listed if the Bruker Engineer has entered it into the configuration of CryoPanel (this requires a service mode password!). The default storage location for logfiles is

    <TOPSPINHOME>/prog/logfiles/cryopanel

Service Login Tab 2.7

The *Service Login Tab* is used for entering a service password. When this tab is selected, the software will issue a challenge number (see Figure 2.7). Based on this challenge number, a Bruker Engineer can issue a temporary password to allow the user access to additional parameters.

After a valid service password has been entered, a red square will appear on the the *Service Login Tab*, where a message indicating that the system is in ‘Service‘ mode or ‘Service (display only)‘ mode will also be displayed. A Logout button also appears. Pressing the Logout button, or exiting out of CryoPanel or TopSpin, will immediately exit back to user mode.

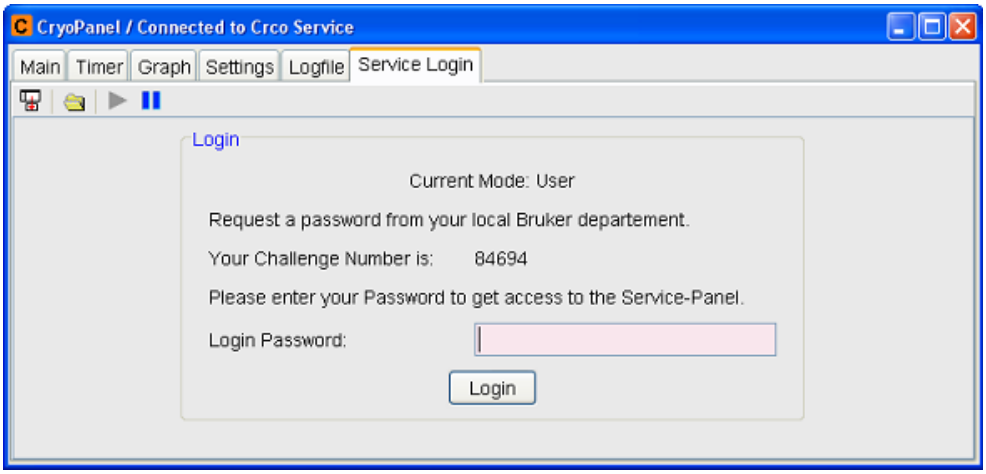

Figure 2.7. Service Login Tab. To obtain a temporary service password, the user needs to forward the ‘Challenge Number‘ to a Bruker CryoEngineer.

Appendix A

CryoPanel Installation A.1

CryoPanel will typically be installed by a Bruker Engineer. For those wishing to install the software on their own, the following steps are provided. If a problem is encountered, please consult the current TopSpin Release Notes for more information.

Hardware Connection A.1.1

The RS232 cable from the cryoplatform must be connected to a free TTY port in the console. This is usually tty07 on an AV or AV/2 console; for an AV/3 IPSO console, it is normally tty04. Note that if tty04 is used for some other accessory on an AV/3 console, a special splitter accessory may be installed. Consult your local Bruker BioSpin Service office for more information.

CryoControl Service A.1.2

The cryocontrol service must be started on the NMR PC. This step typically **needs to be done only once**, unless the service is stopped for some reason. The method for starting the service depends on the PC‘s operating system.

1. LINUX (WS3 or WS4)

    a. Open a shell

    b. Type **`/usr/diskless/crco_data/crco-install`** (if prompted, enter the root password)

    ALTERNATIVELY for LINUX

    a. Open the folder `/usr/diskless/crco_data` in a file browser (e.g. Konqueror)

    b. Double-click `crco-install` (if prompted, enter the root password)

2. Windows (XP Professional, Vista or 7)

   a. open `Bruker Utilities X.Y*->Miscellaneous->CryoControl`. Should this link be unavailable, go to `<DisklessHome>\WinApp`, the default is `C:\Bruker\Diskless\WinApp`

   b. Double-click `w_crco-install`

   * X.Y = TopSpin version, e.g. 3.0

   [To remove CryoPanel: Go to the directory given in 2.a above and double-click `w_crco-remove`]

   SPECIAL NOTE for Windows XP - If the command script shown above fails with an error about a file named ‘MSVCP71.dll‘ and/or ‘MSVCR71.dll‘, there are two possible solutions:

   1) Reinstall the Diskless software which comes on the TopSpin DVD; OR,

   2) Copy the files ‘MSVCP71.dll‘ and ‘MSVCR71.dll‘ from

   `<TOPSPINHOME>/prog/shlib` to `<DISKLESSHOME>/WinApp`, which is often located at `C:\Bruker\Diskless\WinApp`

   After either of these two workarounds, repeat Steps a-b.

3. TopSpin Configuration - Start TopSpin, execute a ‘cf‘, and select the appropriate TTY port (from Step A.1.1) for the Cryo Controller in the list of RS-channels (see Figure A.1).

4. Start CryoPanel - CryoPanel can now be started at any time by typing **`cryopanel`** on the command line of TopSpin. Note that whenever TopSpin is closed, CryoPanel will be closed as well.

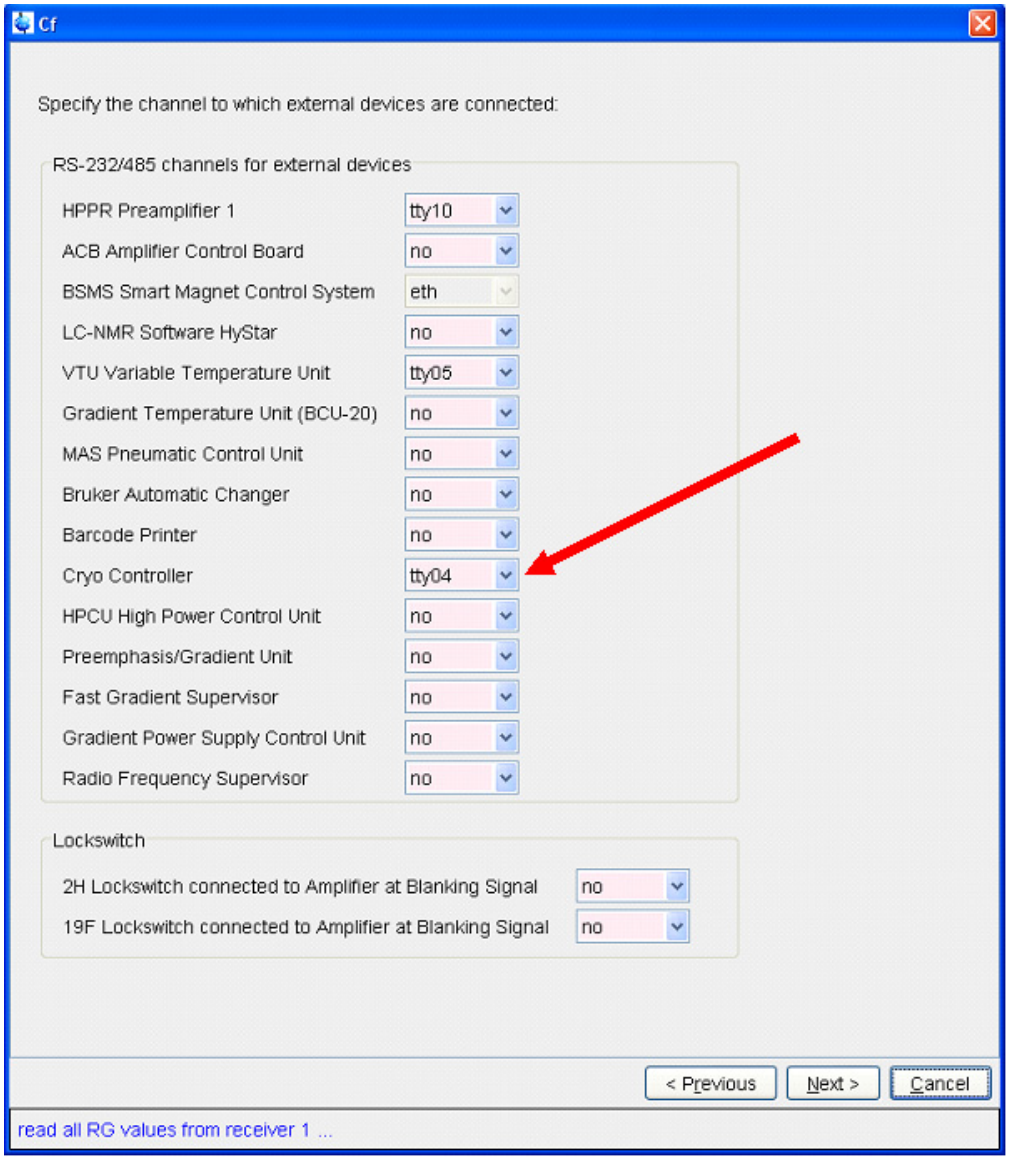

Figure A.1. External Device configuration page of the 'cf" routine in TopSpin, indicating where the Cryo Controller device is connected.

⚠WARNING

Manipulation of the firmware settings can cause serious damage to the Cryoplatform. Changes to the firmware or firmware settings should only be performed by, or under the direction of, an experienced Bruker Engineer.

On systems using CryoPanel, firmware updates and configuration settings for the cryocontroller can be made via the 'standard' UniTool software of TopSpin. (For those familiar with the previous CryoTool software which was installed on a separate laptop, it is no longer necessary to have a separate UniTool program for the CryoProbe™).

Firmware updates can be obtained at

ftp://ftp.bruker.ch/pub/NMR/download/servtools/firmware/crco

To install the update on a PC running CryoPanel, the firmware file must be placed in the directory `<TOPSPINHOME>/conf/instr/servtool/UniTool/files/crco`. If the directory does not exist, then it must be created.

Once the firmware has been downloaded and placed in the correct directory, firmware can be updated as follows:

1. Close TopSpin.
2. Open UniTool:

   Linux - Open a shell and type **`UniTool`**

   Windows - Open `Bruker Utilities 2.1->Service Tools` and Double-click `UniTool` (or `UniTool.cmd`).
3. At the first prompt within UniTool, enter **`crco`** <Return>.
4. Enter <Return> for the address.
5. Select Option `(2) Check/Download CRCO` to have the software check for downloads and update if necessary.
6. If the system detects that an update is necessary, WAIT until the update is complete (~10 minutes). DO NOT make any changes to the computer until it is finished.
7. At the conclusion, a message will appear saying that no updates are necessary (see Figure A.2).

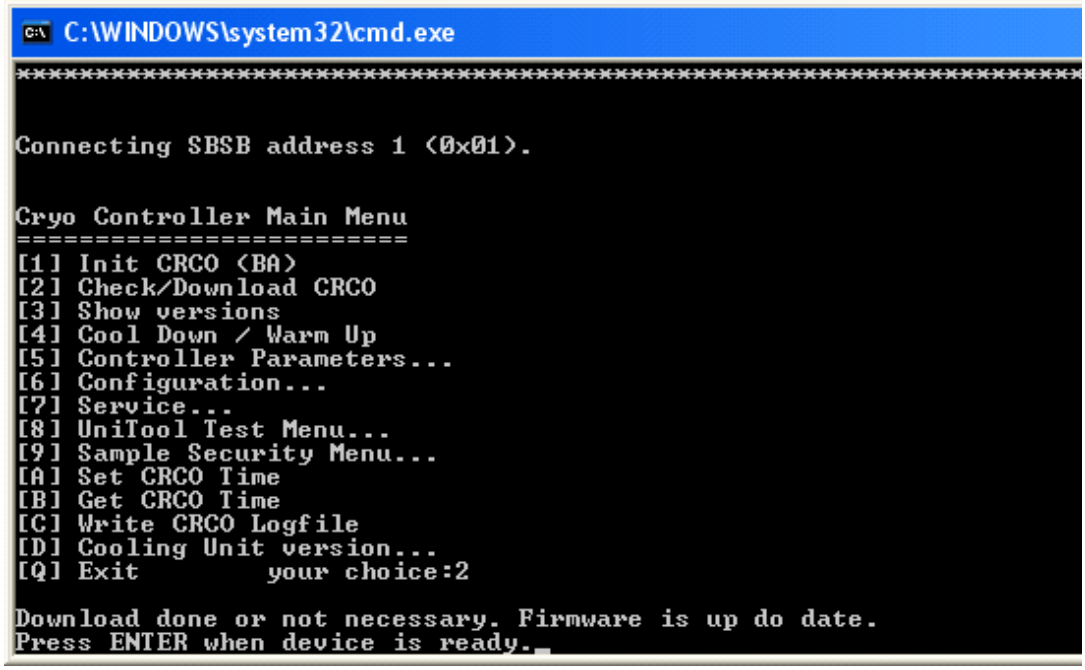

Figure A.2. UniTool display indicating that a firmware update is not needed. This message will also occur at the conclusion of a firmware update.

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