

# **EDTE : VTU Software**

**User manual  
Edte**

**Version 002**

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**BRUKER**

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Manual P/N: Z31464  
DWG-Nr: 1171/ 002

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# ***Index***



# The Edte Software

# 1

Although the Eurotherm controller may be operated manually it is far easier to use the XWIN-NMR software. This enables the value of various parameters, in particular the target temperature, to be set.

For routine use only, the following two operations are regularly carried out :

1. A self-tune is performed.
2. The target temperature is set.

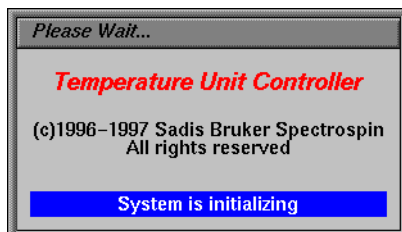
Both operations are most easily carried out using the software.

## Starting EDTE

## 1.1

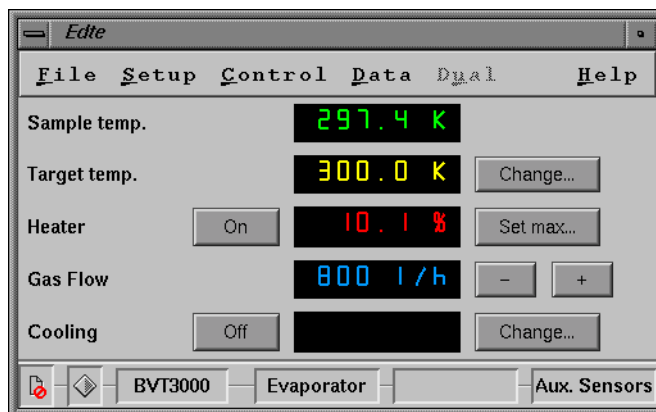
To start the Edte Graphical User Interface, enter **edte** in the **XWIN-NMR** command line. A first window appears, indicating that the program is initializing :

Figure 1.1. Edte Splash Screen



After a few seconds, this window disappears and the Main Window is displayed. It may have different aspects regarding to the connected temperature unit. With a BDTC, BVT3000, or BVT3300, the main window looks like this :

Figure 1.2. Edte Main Window



## Edte Main Window

1.2

The Main Window is divided into three parts :

- The Menu Bar
- The Display Area
- The Status Bar

## The Menu Bar

1.3

The menu bar contains six sub-menus : **Program**, **Setup**, **Control**, **Data**, **Dual** and **Help**.

## The File menu

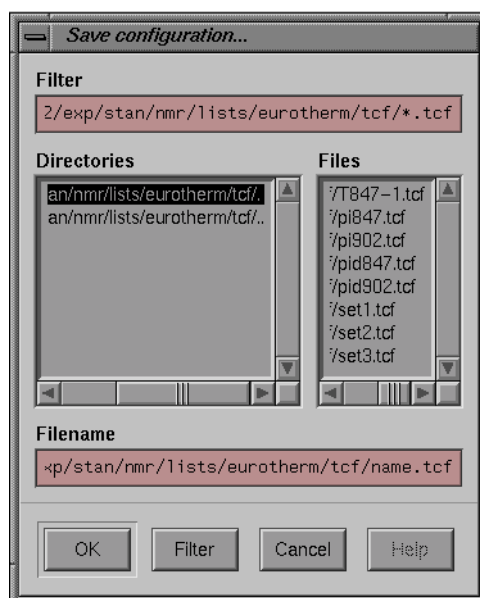
1.3.1

### Save configuration...

Creates a configuration file (\*.tcf) used to store some parameters of the temperature unit such as Target, Max Output-Power, Gas Flow and Self-Tune settings (Proportional Band, Integral and Derivative time).

The file is located in the **/u/exp/stan/nmr/lists/eurotherm/tcf** directory. The user has only to give a name to the configuration file in this window :

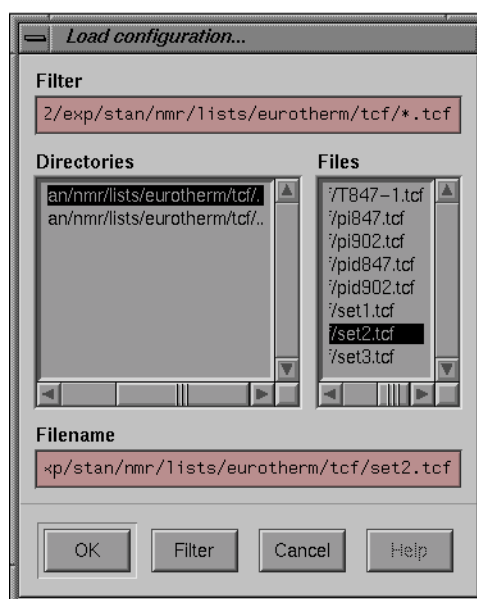
Figure 1.3. Save Configuration Window



### Load configuration...

To reload the parameters saved in a tcf file. A directory browser shows the available files :

Figure 1.4. Load Configuration Window

**Download to temperature unit**

Activating this menu will allow to update the software of the BVT3000 or BVT3300 mainboard. Edte asks for the NMR-superuser (or root) password to begin the process.

***This menu should only be used by the Bruker Service Engineers.***

Figure 1.5. Download Window



In the download window, the user will have to select a file in the proposed list, and click the start button to begin the download process. The files are located in the ***/u/exp/stan/nmr/lists/eurotherm/hex*** directory.

While downloading, the program displays the percentage already transferred.

At the end, the windows informs the user that the download was successful.

As this function is only available on a BVT3000 or 3300, the menu is grayed if another model is detected.

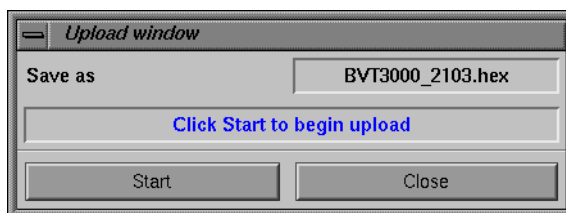
**Upload to temperature unit**

As it is possible to download, it is also possible to upload the software of the BVT3000 or BVT3300 mainboard in order to save the software.

Edte asks for the NMR-superuser (or root) password to begin the process.

***This menu should only be used by the Bruker Service Engineers.***

Figure 1.6. Upload Window



Edte automatically generates a file name and the user has just to click the start button to begin the upload process. The total number of bytes already uploaded is displayed while uploading.

At the end, the window informs the user that the upload was successful.

The files are located in the /u/exp/stan/nmr/lists/eurotherm/hex directory.

As this function is only available on a BVT3000 or 3300, the menu is grayed if another model is detected.

### **Exit**

Quit the program.

## **The Setup Menu**

### **1.3.2**

### **Units**

Allows the user to select the desired temperature unit (Celsius, Kelvin, Fahrenheit). The currently active temperature unit is marked. Not available temperature units are grayed.

### **Sensors**

Choose the sensor you have connected. Only the available sensors are proposed, others are grayed.

### **Display**

Set the decimal precision to 0, 1, or 2 digits. Unavailable for most temperature controllers.

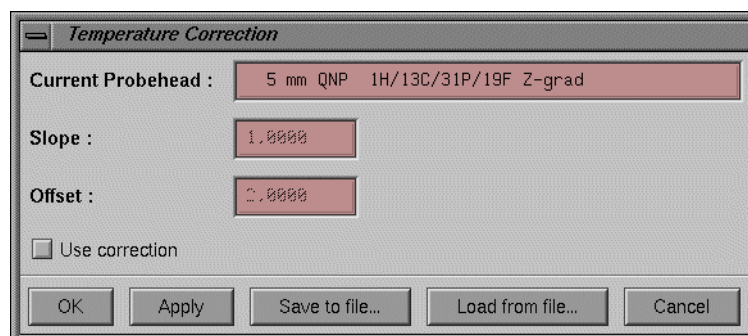
### **Lock front**

This toggle button enables or disables the front key access.

**Temperature correction...**

This menu displays the following window :

Figure 1.7. Temperature Correction Window



For information, the current probehead is displayed.

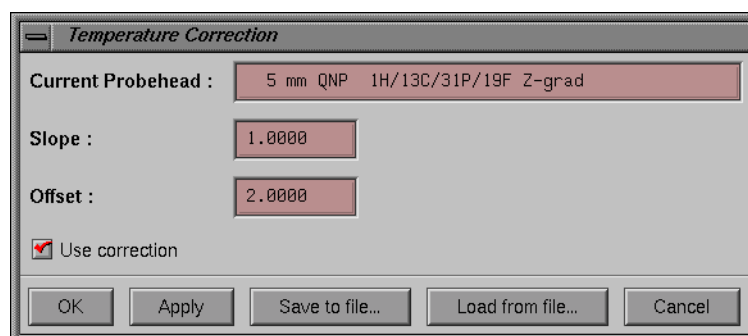
In this window, you can define if a correction must be applied, and set the offset and slope values. To apply the new values, use the Apply or OK button.

If correction is used, the Eurotherm target is recalculated in the following way :

$$\text{EurothermTarget} = \text{Slope} \times \text{SampleTarget} + \text{Offset} \quad (\text{Eq. 1.1})$$

The corrections can be saved or recalled from a correction file using the **Save to file...** and **Load from file...** buttons. The correction file contains the Slope and Offset values, and if the correction is used or not. The probehead id and description are also saved. When recalling a correction file, edte verifies that the current probehead matches the saved one, and asks for a user confirmation if not.

Figure 1.8. Temperature Correction is used



In this example, the user has defined a 2 degree offset between the Sample and the Eurotherm Target temperature. If he sets the Sample Target temperature to 320 Kelvin, the eurotherm will be programmed to reach 322.

When correction is used, a toggle button in the status bar of the main window changes color to blue. When no correction is applied, the toggle button is grayed as shown in the following pictures :

Figure 1.9. Correction is used (The toggle button is blue)



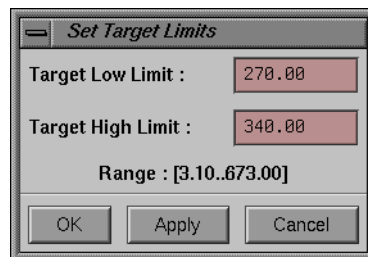
Figure 1.10. No Correction (The toggle button is gray)



## Target-Limits...

This menu allows to set the range of valid Target temperature in order to avoid probehead damages. The user has to defined the high and low limit. These values must fit into the sensor temperature range.

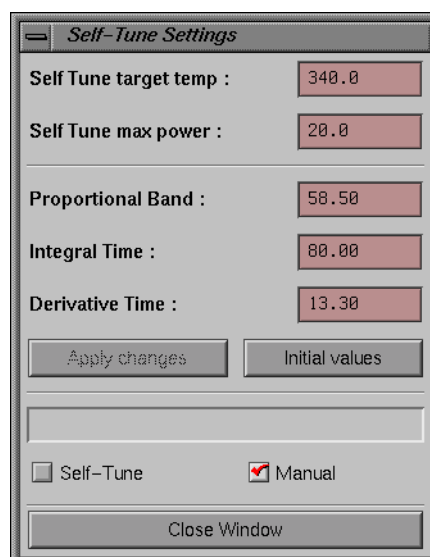
Figure 1.11. Target Limit Window



## Self-Tune...

This menu displays the Self-Tune window :

Figure 1.12. Self-Tune Window



To perform a self-tune, just give the Self-Tune target temp, and the max output power. The self-tune will be started when the Self-Tune toggle button is set. It can be interrupted by activating the manual button. In manual mode, you can change the Proportional Band, Integral and Derivative Time values and apply with the Apply Changes button. Initial Values will reload the original Proportional Band, Integral and Derivative time (P.I.D.) values.

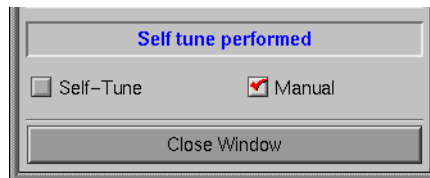
When the self-tune is running the status bar shows the following message :

Figure 1.13. Self Tune is running



When the self-tune is finished the new P.I.D. values are loaded and the status bar shows the following message :

Figure 1.14. Self-Tune is performed



## Cutback...

Overshoot and undershoot can be eliminated by the correct setting of cutback low and cutback high. The values are automatically set when a self-tune is performed.

Figure 1.15. Cutback Window



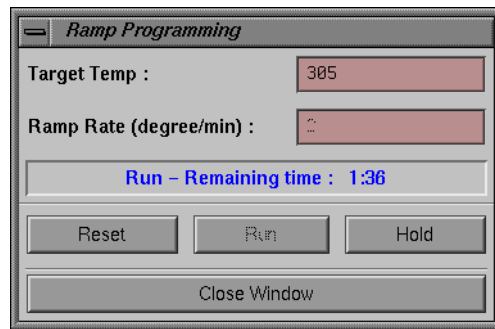
## Adaptive Tune

This toggle button menu allows to switch from a fixed P.I.D. based regulation to a adaptive tune regulation. This feature will overwrite the parameters P,I and D when a disturbance indicates that they are incorrect.

## Ramp...

This menu enables the use of ramp functions :

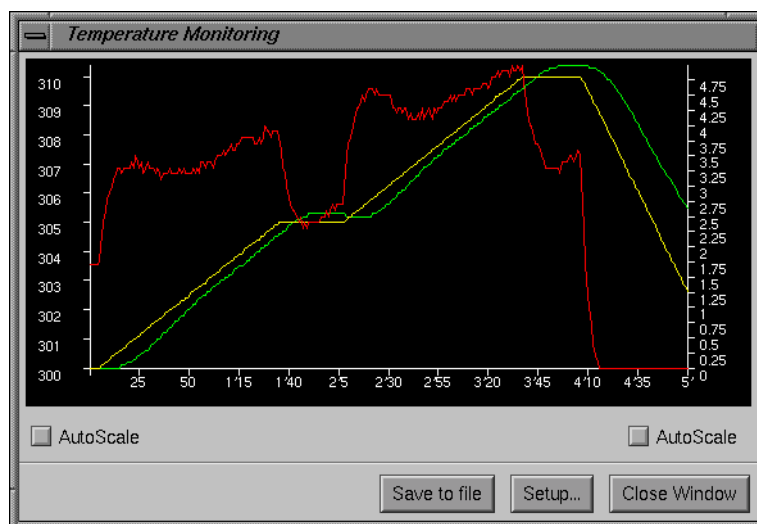
Figure 1.16. Ramp Window



To use ramps, the user has to define the temperature to reach and the speed. Then click the **Run** button to start the ramp. The **Reset** stops the ramps (switch to P.I.D. mode). The status bar displays the remaining time. While the ramp is running, the user may change the target by entering a new value and hit the return key.

The Monitor Window displays a 3 segment ramp with different Ramp Rate :

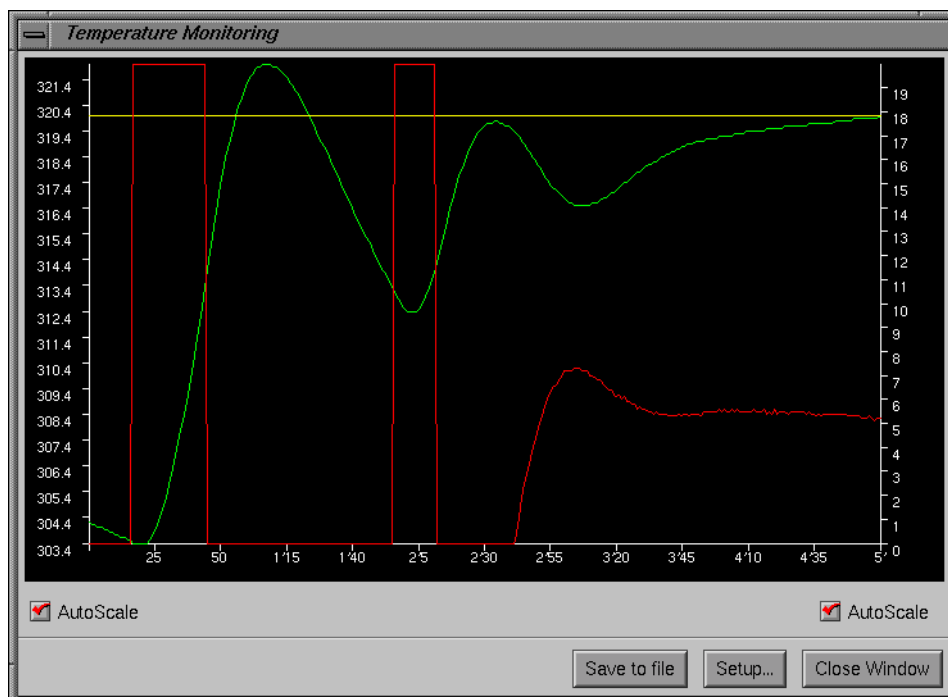
Figure 1.17. Monitoring Ramps



**Monitor temperature and Output Power**

This menu displays a window containing a graphical tool that displays the evolution in the 2 last minutes of sample and target temp, and output power. One point is taken every second. This setting can be modified with the **Setup...** button.

Figure 1.18. Monitor Window



The **Save to file** button performs a quick data saving to disk in a file located in the **/u/exp/stan/nmr/lists/eurotherm/record** directory. The name is generated automatically using the following pattern : **myyyymmdd-n.rec** where **yyyy** is the year, **mm** the month, **dd** the day and **n** and incremental number :

Table 1.1. Example of AutoSave Generated Filename

m19970715-1.rec	m19970715-2.rec	m19970715-3.rec
m19970715-4.rec	m19970715-5.rec	m19970715-6.rec
m19970715-7.rec	m19970715-8.rec	m19970715-9.rec
m19970715-10.rec	m19970715-11.rec	m19970715-12.rec
m19970716-1.rec	m19970716-2.rec	...

These files can be viewed using the **Display Recorded Datas...** menu.

The scale is automatically calculated but the user may change these values. To change the temperature scale, move the mouse pointer to the Temperature Axis and press the left mouse button. Move the mouse to define the region to zoom in on. A gray rubber band shows the delimited region. Release the mouse button to

zoom the area. To zoom in on the output power, follow the same process on the right axis.

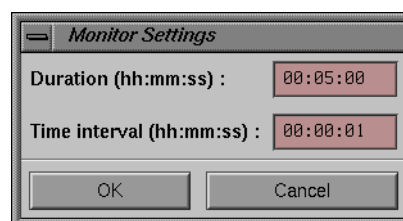
To go back to automatic scale, click the toggle button **AutoScale**.

With the right mouse button, a menu can be activated. It displays informations about the current Graphic Display Settings (Duration and Interval). This menu also displays the name of each displayed sensor. Toggle buttons, associated to the displayed sensors, can be set (unset) to show (hide) the curve.

### **Monitor settings**

This menu displays a window for setting the monitor parameters.

*Figure 1.19. Monitor Setting Window*

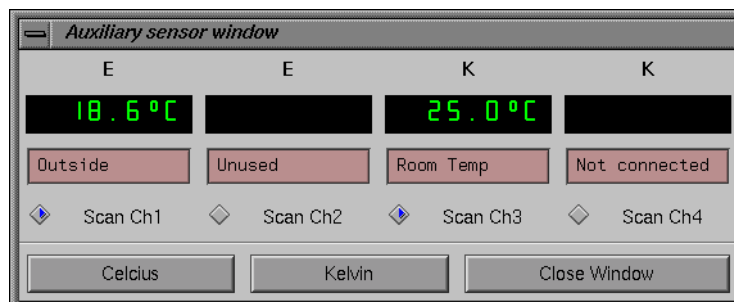


Set the Monitor duration using the hh:mm:ss or HHh MMm SSs format (00 :10 :00 or 10m). Time Interval defines the interval between two temperature acquisitions.

### **Auxiliary sensor module**

This menu displays the Auxiliary sensor module window.

*Figure 1.20. Auxiliary Sensor Module Window*



It displays the sensor type, the measured value, and the scan status. Only the scanned channels are displayed. It is possible to switch from Celcius to Kelvin units. A description can be assigned to each channel.

**Record Settings...**

Recording allows to store in an ASCII file, several parameters values concerning the temperature unit at a given time interval.

The recording status is displayed in the status bar of the main window :

*Figure 1.21. State 1 (No settings for recording)*



*Figure 1.22. State 2 (Record can be started / is stopped)*



*Figure 1.23. State 3 (Recording is active)*



The user has to set the filename, the time interval between two points, general informations and the parameters to store :

Time Interval can be entered using the HH :MM :SS or HHh MMm SSs format. Standard time intervals are proposed by Edte when clicking the right button over the Time Interval text field.

When the settings are applied the record bitmap indicator of the main window status bar changes from 1 to 2. If the file already exists, the user has to confirm that he wants to overwrite the file. The files are located in the /u/exp/stan/nmr/lists/eu-rotherm/record directory.

**Start Recording**

Starts recording, the bitmap indicator changes from 2 to 3. Recording can also be started by clicking the bitmap in the state 2.

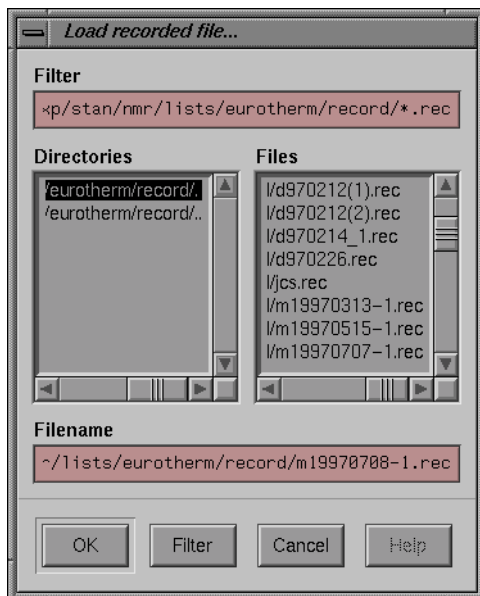
**Stop Recording**

Stops recording, the bitmap changes from 3 to 2. Recording can be stopped by clicking the bitmap in the state 3.

## Display recorded datas...

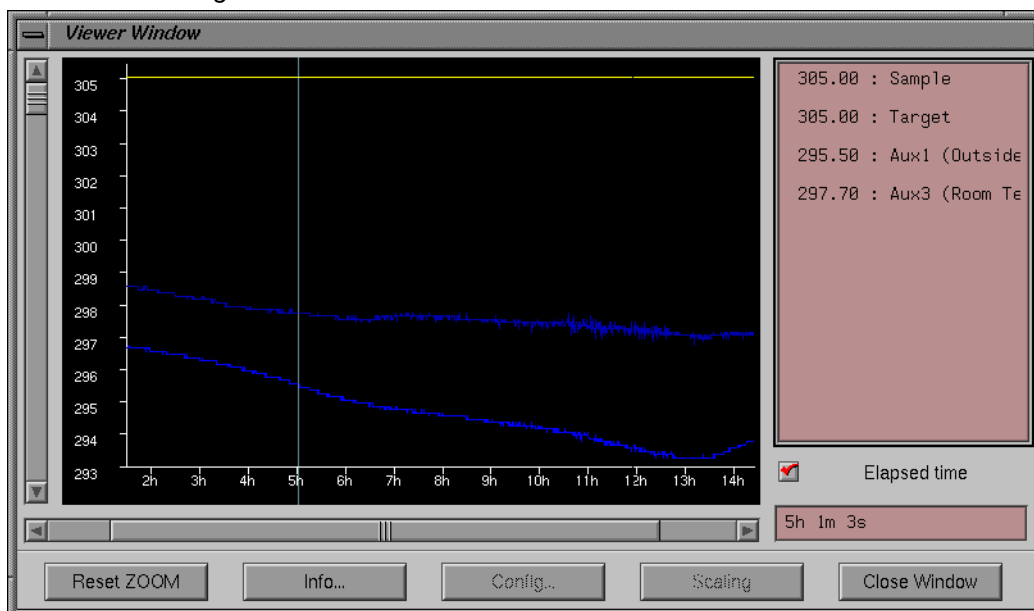
Recorded Datas can be displayed with a viewer. The user has to select the record file using the file browser :

Figure 1.24. Load Recorded File Window



When a file is selected, a viewer, similar to the Monitor, appears.

Figure 1.25. Viewer Window



When moving the mouse over the series of points, a vertical axis is displayed. The (Elapsed/Absolute) time and the sensor values and description are displayed in the right part of the screen. Time can be displayed as elapsed (First point is taken as time reference) or absolute time (Date is also displayed).

The viewer allows zooming on the x and y axis using the mouse. Press the left mouse button in the background and drag to define the interest area. Release the mouse button to define the zoom area. Use the horizontal and vertical scrollbar to move the interest area.

To reset the zoom, click the **Reset Zoom** button.

The **Info...** button displays a window containing informations about the record file (date, time, user, comment).

The user can enable or disable a serie of point in the popup menu attached to the right mouse button.

This menu is available if the connected temperature unit is a BEST.

With a BEST, the main window has additional informations to control the second eurotherm :

Figure 1.26. The Main Window enhanced in BEST mode



The buttons work the same way as for a standard temperature unit with one eurotherm.

Some special settings are common to both eurotherm and automatically send to the **Liquid** and the **Probe** controller using the **Setup** menu. If a functionality was specific to the second eurotherm, its menu has been placed in the **Dual** menu.

By changing the temperature unit (Celsius, Kelvin, Fahrenheit) in the **Setup** menu, the **Probe** and **Liquid** eurotherm are affected.

### **Target-Limits...**

This menu allows to set the range of valid Target temperature in order to avoid probehead damages. The user has to defined the high and low limit. These values must fit into the sensor temperature range.

### **Self-Tune...**

This menu displays the self-tune window allowing to perform an automatic self-tune or to change manually the P.I.D. values.

### **Cutback...**

Overshoot and undershoot can be eliminated by the correct setting of cutback low and cutback high. The values are automatically set when a self-tune is performed.

### **Display**

Set the decimal precision to 0, 1, or 2 digits.

### **Lock front**

This toggle button enables or disables the front key access.

## The Help menu

1.3.6

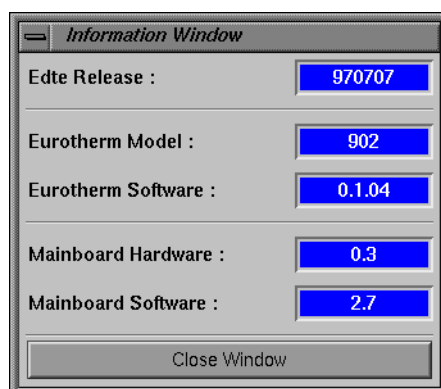
This menu contains informations about how to reach us.

Comments and suggestions are welcome. Please send your request to the support email : [nmr.software@bruker.fr](mailto:nmr.software@bruker.fr)

### **Display informations...**

Activating this menu will display informations about Edte, the Eurotherm, and the MainBoard (if available).

Figure 1.27. Information Window



### **Edte User's Manual (pdf)...**

Displays this manual with Acrobat Reader.

## The Display Area

1.3.7

The display area contains the most important informations coming from the temperature unit :

- The sensor temperature
- The target temperature
- The heater power / state
- The gas flow level / state
- The cooling power / state

and several buttons to setup and activate different temperature unit functions :

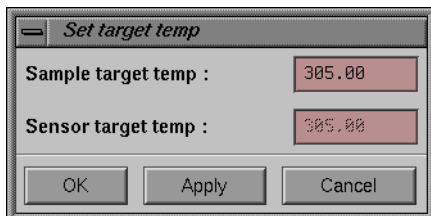
- Setting target temp
- Start / Stop heating
- Setting max power
- Increase / decrease gas flow level
- Start / Stop cooling
- Setting cooling power

## Changing the target temp

To change the target temp, click the Change button near the Target Temp value (the yellow one).

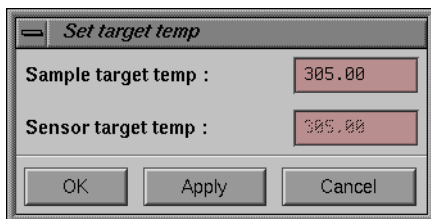
The following window will appear :

Figure 1.28. Set Target Window



Enter in the Sample Target Temp field, the desired temperature. If temperature correction is used, a new value will be calculated in the Sensor Target Temp field. This value will be applied.

Figure 1.29. Set Target Window



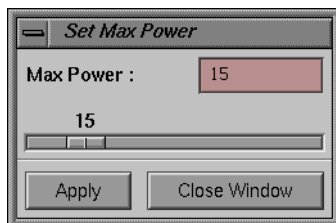
## Starting / Stopping heating

To start / stop heating, click the button at the left of the output power value (the red one). Its label will switch from **Off** to **On**. If the power is switched off due to missing gas flow, the label will show the heater status (switch to Off without user interaction). If there is overheating, the output power will contain a blinking error message **OVERHEAT**.

## Changing the Max Output Power

To change the High Power Limit, click the **Set Max button**, or use the right mouse button, on the output power. The right mouse will display values in a list in 5% step. Select a value. In the Max Power Window, use the scale bar, or enter the value in the text box. **Apply** the changes and **Close** the window.

Figure 1.30. Set Max Power Window



***Changing the gas flow***

To change the gas flow, use the + or - button. Another possibility is to use the right mouse button on the displayed value. A list of 16 values will appear. Just select the desired gas flow.

If there is no gas flow, the blinking error message **MISSING** will appear instead of the gas flow level.

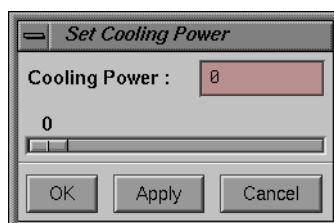
***Starting / Stopping cooling***

Same as for Heating.

***Changing the cooling power***

Same as for Heating :

*Figure 1.31. Set Cooling Power Window*



The Cooling display is also used to inform the user about the LN2 level. Instead of the cooling power, a **REFILL** or **EMPTY** message may be displayed :

The status bar displays information about recording, temperature correction, the temperature unit type and the availability of some options, like evaporator, exchanger, auxiliary sensors module and booster.

*Figure 1.32. No settings for recording*



*Figure 1.33. Record can be started / is stopped*



*Figure 1.34. Recording is active*



*Figure 1.35. No correction is applied (gray)*



*Figure 1.36. Correction is active (blue)*



The Eurotherm controller is used to monitor and control the temperature of the gas flow surrounding the sample. To do this optimally it needs to measure how the system responds to changes in the regulation heater power. The required information is obtained during the self-tune routine. If a proper self-tune is not carried out, then the system will be slow to reach equilibrium and there may be a large overshoot or undershoot when a new target temperature is set.

## ***What is a self-tune***

## **2.1**

A tuning is necessary to match the characteristics of the controller to that of the process being controlled in order to obtain good control. This means :

1. Stable control of the temperature at the setpoint without fluctuation
2. No overshoot or undershoot
3. Quick response to deviation from the setpoint.

Self-tune involves calculating and setting the values of the P.I.D. parameters :

### ***Proportional Band (P)***

The Proportional Band is the bandwidth over which the output power is proportioned between 0 and the max power. Outside this bandwidth, the max power is applied.

### ***Integral Time (I)***

Determines the time taken by the controller to remove steady-state error signals.

### ***Derivative Time (D)***

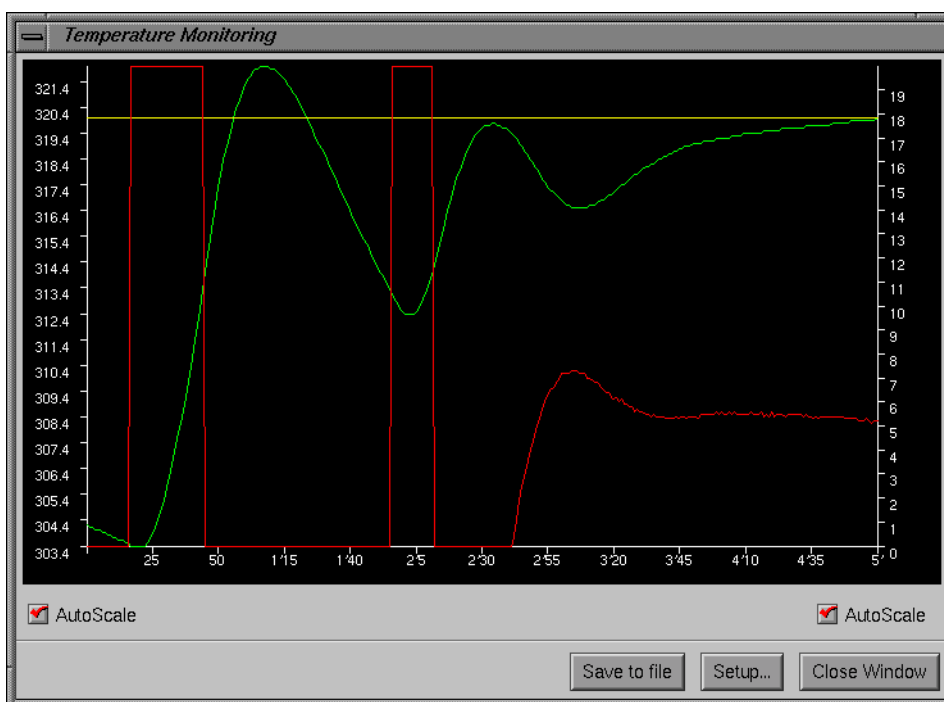
Determines how strong the controller will react to the rate-of-change of the measured value.

## ***Self-Tune process***

## **2.2**

The regulation heater is switched on at maximum power (subject to the setting of HO - high output) for one or several short periods of time. The Eurotherm controller measures the response of the system to this power. From the response, three parameters TI, TD and XP (P.I.D. parameters) are automatically calculated and set.

Figure 2.1. Self-Tune process



A further parameter (LB overshoot limitation) may also be set, if the range over which the self-tune is carried out is sufficiently large.

## When should a self-tune be carried out ?

## 2.3

Initially when the system is installed, or, whenever a significant change in the operating conditions is made.

### **Changes that warrant reactivating self-tune are :**

1. Changing the rate of flow of input gas as displayed on the BVT3000 front panel.
2. Large changes in temperature of input gas. Minor temperature fluctuations caused by room temperature changes will not upset the temperature regulation.
3. Altering the position of the thermocouple.
4. Exchanging a probe.
5. Changing the target temperature by more than 10 K.

### **Changes that do not require reactivating self-tune :**

1. Changing the sample.
2. Changing the target temperature by less than 10 K.
3. Turning sample spin on or off.

## How to perform a self-tune

## 2.4

1. The self-tune should be carried out under the exact conditions of operation. Insert the heater, thermocouple and sample. The heater can be switched on but first ensure that the target temperature is not too high. If a cooling unit or N<sub>2</sub> heater are to be used, then they should be operating normally. Ensure that the gas flow is attached to the probe base. If the experiments are normally carried out with spinning samples, then the sample should spin during the self-tune.
2. Enter the command "edte".
3. Be sure the heater is on and click the **Control - Self-Tune** menu to activate the Self-Tune Window :

Figure 2.2. The Self-Tune Window

4. The self-tune target is set to the current target temperature. This value can be changed. The self-tune max power is set to the current Output Power. It may also be changed.
5. Start the self-tune process by clicking the **Self-Tune** toggle-button. **Self-Tune is running** is displayed in the status-bar. Clicking the **Manual** toggle button will stop the self-tune process.
6. When **Self-Tune is performed**, the values of XP, TI and TD are loaded. These values may be changed manually and applied with the **Apply changes** button.
7. The new target temperature is automatically set to the Self-tune target temp and regulation is active.

*It is possible to have Proportional only, or 'PD' or 'PI' control. Just set the Integral or/and Derivative time to 0.0 before starting a self-tune. The tuner will leave them off and will not calculate a value for them.*

### *How to store temperature parameters*

2.5

Different operating conditions may require different P.I.D. parameters. For example, two types of routine experiments may be regularly carried out, room temperature work with a 5mm probe and low temperature work with a 10mm probe.

It is possible to store the two sets of edited parameters in two separate files which can quickly be loaded.

#### *Save a set of temperature parameters*

2.5.1

1. Enter Edte.
2. When a suitable set of parameters has been set, use the menu **File - Save Configuration...**
3. In the browser, type in a new name (e.g. 10mmLOW) and press **OK**. The parameters are stored in the file 10mmLOW.tcf in the **/u/exp/stan/nmr/lists/eurotherm/tcf** directory,

Some operators prefer to carry out a self-tune each time a probe is changed and do not keep a set of stored parameters.

#### *Read in a set of temperature parameters*

2.5.2

1. Enter "edte".
2. Click on **File - Load Configuration...** menu
3. The browser will display the stored files. Select the one to be loaded and click **OK**.

### *Adaptive Tune*

2.6

For routine work, it is recommended that you operate with ADAPTIVE TUNE set to "off". Adaptive tune is designed for systems that experience changing conditions e.g. change in rate of air flow, change in input air temperature etc. Such variations are not normal for routine NMR work and so adaptive tune should not be required.

However, if you wish to ensure that the P.I.D. parameters are constantly monitored and optimized then there may be an advantage to working with ADAPTIVE TUNE set to "on" by activating the **Control - Adaptive-Tune** check menu.

The sensor does not directly measure the sample temperature but the temperature just below the sample. There might be a difference between the real sample temperature and the measured value. Batman has been developed in order to determine the eurotherm target temperature in order to have the desired temperature in the sample.

Batman is an AU program, launched from within XWIN-NMR, that automatically calculates this temperature difference. The process may need several steps :

1. Set initial eurotherm target temperature to the desired sample temp
2. Set the temperature
3. Wait for stabilization
4. Compute the real sample temperature using the chemical shift
5. Compute the new eurotherm target temp
6. repeat steps 2..5 until the desired sample temperature is reached

In order to perform this set of calculations, BATMAN first requires the input of several fundamental parameters :

**Target temperature** in K (the desired probe temperature)

**Stabilization time** in seconds (the minimum period of thermal stability that must elapse before data are acquired)

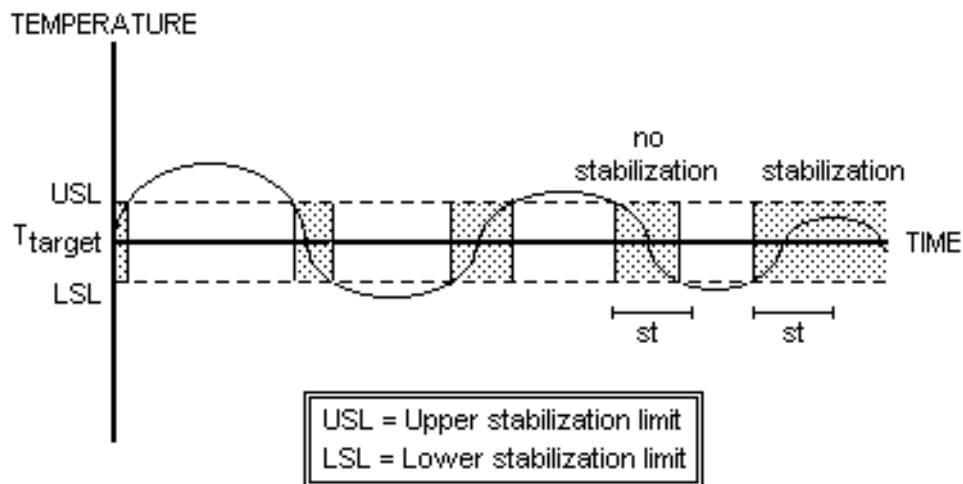
**Precision** (the maximum amount of temperature fluctuation allowed above and below the target temperature -- the temperature is considered «stable» when within this range)

**Sample type** ((G)lycol or (M)ethanol)

**Sample origin** ((P)ure MeOH/Glycol or (B)ruker MeOH/Glycol sample)

The final entry made by the user is a «CR» when the sample has been introduced into the spectrometer. Subsequently, BATMAN, picks the appropriate peaks from the acquired spectrum and stores the chemical shift difference in the file peaklist. Additional chemical shift measurements, made using this program, are stored in the same file. These values are processed to generate the linear systems used to correlate sample temperature to target/probe temperature.

Figure 3.1. Thermal stabilization process



The curve shows a diminishing thermal fluctuation until stability around the target temperature is achieved. Shaded regions represent times at which stabilization occurs. These times must be longer than the prescribed stabilization time (st) in order for a signal to be acquired.

Factors that slow the signal acquisition process are :

- i) prescription of a long stabilization time
- ii) prescription of a narrow precision window

# Directories and File Formats

# 4

## Edte Directories

## 4.1

Edte uses 5 directories all located in `/u/exp/stan/nmr/lists/eurotherm`.

- config

This directory contains configuration files used internally by edte.

***The user should not modify these files.***

- hex

This directory contains HEX files. These files are used to update the Variable Temperature Unit firmware.

***These files are reserved to the Bruker Service Engineers.***

- corr

This directory contains the correction files generated by the **Save to file...** button in the **Temperature Correction** window. They have all the same extension (.cor). The same directory is used to display the available file to load a temperature correction parameter set.

- record

This directory contains the record files generated by the Monitor or the Record feature included in Edte. All files have the same extension (.rec).

- tcf

This directory contains the Variable Temperature Unit configuration files generated by the **File - Save Configuration...** menu. The same directory is used to display the list of available files when the **Load Configuration...** menu is activated.

## Edte Files

## 4.2

### Record Files

### 4.2.1

The Record Files format is similar to the Microsoft INI files format. It is divided into sections, and each value is assigned to a Key.

A Record File contains 4 sections :

### **Info Section**

This section contains general informations like **User** and **Title**, but also **Date**, **Time** and the data **Source**.

### **Cols Section**

This section describes which sensors are stored. C1 (**Date**), C2 (**Time**) and C3 (**Elapsed Time**) are always present.

### **AuxSensors Section**

When auxiliary sensor are used, their name and Type are stored.

Aux?Desc is the description of the sensor

Aux?Type is the sensor Type (T, K, E, Pt100)

? = 1,2,3 or 4

### **Data Section**

The data section contains the sensor values. They are stored from left to right and correspond to the sensors defined in the cols section. The first column is C1 (**Date**), the second one is C2 (**Time**), the third one is C3 (**Elapsed Time**) and so on.

### **Example**

```
[Info]
Source=xTempRecording
Date=07/08/1997
Time=14:30:03
User=Patrice
Title=Long Time Stability Test
```

```
[Cols]
C1=Date
C2=Time
C3=Elapsed Time
C4=Sample
C5=Target
C6=Output Power
C7=Aux1
C8=Aux2
C9=Aux3
C10=Aux4
```

```
[AuxSensors]
Aux1Desc=Outside
Aux1Type=E
Aux2Desc=Unused
Aux2Type=E
Aux3Desc=Room Temp
Aux3Type=K
Aux4Desc=Not connected
Aux4Type=K
```

```
[Data]
08/07/1997  14:30:09    6   300.00 300.00 1.60  23.40  25.30  25.20 1372.00
08/07/1997  14:30:14   11   300.00 300.00 1.70  23.40  25.30  25.20 1372.00
08/07/1997  14:30:19   16   300.00 300.00 1.70  23.40  25.30  25.20 1372.00
```

08/07/1997	14:30:25	22	300.00	300.00	1.60	23.40	25.30	25.20	1372.00
08/07/1997	14:30:30	27	300.00	300.00	1.50	23.40	25.30	25.20	1372.00
08/07/1997	14:30:35	32	300.00	300.00	1.70	23.40	25.30	25.20	1372.00
08/07/1997	14:30:40	37	300.00	300.00	1.50	23.40	25.30	25.20	1372.00
08/07/1997	14:30:46	43	300.00	300.00	1.60	23.40	25.30	25.20	1372.00
...									

## TCF Files

## 4.2.2

A TCF file contains several informations about the Variable Temperature Unit. These files are generated when using the **File - Save (Load) Configuration...** menu.

Two section are used to store the VTU parameters.

### Version

This section identifies the Variable Temperature Type. A BVT3000 tcf file may not be compatible with a BDTC tcf file. The software checks the version type.

### Parameters

This section contains the parameters of the Variable Temperature Unit.

The setpoint value is associated to the **SP** parameter.

**HO** represents the Max Output Power (0-100).

**AF** is the value of the GasFlow (0-15).

**NH** is the nitrogen heater power (0-100%).

**XP, TI, TD** are the PID values.

All these values can be set using the Edte Graphic User Interface.

***There is no way to add other parameters to a tcf file. If it is necessary to add other parameters, modifications must be done in the software.***

### Example

[Version]

Version=BVT3000

[Parameters]

SP=320.00

HO=20.00

AF=6

NH=-1

XP=68.40

TI=160.00

TD=26.70

### Compatibility

***Files stored with a previous version of Edte (before XWin-NMR 2.0) cannot be loaded with this new version of the software.***

The user will have to create new tcf files.

As previous parameter files are ASCII files, it is possible to print them from a unix-shell. They are located in the **/u/exp/stan/nmr/lists/eurotherm** directory and have the following format :

```
SL 303.3
HO 20.0
TI 10.0
TD 1.7
HB 7.6
LB 26.3
XP 5.3
HP1
NP0
BP 0.0
RR 0.0
TR 17.0
S2 298.0
OS> 0
XS> 4
```

**XP, TI, TD** are the PID values. They can be manually entered in the Self-Tune Window.

**SL** is the setpoint (**SP**)

**HO** is the Max Output Power.

**NP** is the Nitrogen Power.

### **toEdte**

Another solution is to use the toEdte PerlScript to convert older parameter files. This script is located in **/u/exp/stan/nmr/lists/eurotherm**.

The Syntax is :

```
toEdte <parfile>
```

This PerlScript converts the file <parfile> to a new file parfile.tcf located in the tcf sub-directory. It extracts the XP, TI, TD, SP , HO, NP from the older file and generates a new parameter file compliant with the new structure.

## **Correction files**

### **4.2.3**

Correction files are used to store the temperature corrections parameters as set in the **Temperature Correction...** menu. They are saved in the **/u/exp/stan/nmr/lists/eurotherm/corr** directory.

### **Parameters**

This file contains two sections : [ProbeHead] and [Correction].

The [ProbeHead] section contains the Id and Description of the current probehead as set with **edhead**. A warning is displayed if the user wants to load a correction file which probehead does not match the current one.

The [Correction] section contains the correction parameters (Offset and Slope) and the flag indicating it is enabled or not (Corr = On or Off).

**Example 1**

This example show the correction file when Correction is disabled.

```
[ProbeHead]
Id=7
Desc= 5 mm QNP 1H/13C/31P/19F Z-grad
```

```
[Correction]
Corr=Off
Slope=1.00000
Offset=0.00000
```

**Example 2**

This example shows a linear correction of 2 degrees

```
[ProbeHead]
Id=7
Desc= 5 mm QNP 1H/13C/31P/19F Z-grad
```

```
[Correction]
Corr=On
Slope=1.00000
Offset=2.00000
```

With this set of correction applied, a sample target temperature of 320K will be send to the Eurotherm as a 322K sensor target temperature.



# AU Program and Command Line instructions

# 5

## Using the XWin-Nmr command line

5.1

One parameter and four commands are available to the user to interact with the temperature unit within an AU program or using the XWin-Nmr command line.

### The TE parameter

5.1.1

#### **TE is always in KELVIN**

TE contains the last target temperature applied or to be applied to the eurotherm.

In the following two lines :

```
te 320.0
```

```
teset
```

the TE parameter is set to 320.0K and its value is applied as the new target temperature..

The following two lines :

```
teget
```

```
ls TE
```

display the current sample temperature loaded with TEGET.

### TESET

5.1.2

This command allows the user to send the value stored in TE to the temperature as the new target temperature.

#### **Syntax :**

```
teset
```

or

```
teset temp
```

When **TESET** is used without parameters, **TE** is used,

### TEGET

5.1.3

This command loads the TE parameter with the current target temperature.

**Syntax :**

```
teget
```

The command **1s TE** displays the value loaded with TEGET.

### TEREADY

5.1.4

This command waits for a stabilisation time after that the defined precision has been reached.

**Syntax :**

```
teready Stabilisation_Time Precision
```

This command is used in conjunction with **TESET** in the following way (xwin-nmr command line) :

```
teset 320.0
```

```
teready 300 0.5
```

The target temperature will be set to 320K and **TEREADY** will wait additional five minutes (300 seconds) after the measured temperature had been 10 seconds in a 0.5K stabilization range (319.5 .. 320.5).

### TEPAR

5.1.5

This command loads a parameter file previously stored with Edte using the **File - Save Configuration...** menu.

**Syntax :**

```
tepar
```

or

```
tepar file.tcf
```

When no parameter file is specified, the list of available parameter files are displayed in a list. Click a filename to apply its values.

## Using an AU Program

5.2

All the above described function can be included in an AU Program. The syntax is a little bit different for some commands.

**The TE parameter****5.2.1****Setting TE**

```
STOREPAR("TE", value);
```

**Reading TE**

```
FETCHPAR("TE", &value);
```

where **value** is a float.

**Reading the Sample Temperature**

To read the Sample Temperature use FETCHPARS instead of FETCHPAR after a TEGET command :

```
TEGET;

FETCHPARS("TE", &value);
```

**TEGET****5.2.2****Syntax :**

```
TEGET;
```

**If a compilation error occurs use the following line instead of TEGET :**

```
{ SETCURDATA AUERR=CPR_exec( "teget", WAIT_TERM); }
```

**TESET****5.2.3****Syntax :**

```
TESET;
```

**TEREADY****5.2.4****Syntax :**

```
TEREADY(Stability_Duration, Precision);
```

where **Stability-Duration** is an integer, and **Precision** a float.

**TEPAR****5.2.5****Syntax :**

```
TEPAR(filename);
```

where filename is a string variable or constant string.

The following AU Program

```
...  
STOREPAR("TE", 320.0);  
TESET  
TEREADY(300, 0.5)  
TEGET  
Proc_err(1, «Sampe Temperature is : %.2fK.\n», fTE);  
...
```

sets the target to 320.0K, waits for a 5 minutes stabilization time after a precision of +/-0.5K and displays the reached Sample Temperature.

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