The list of the control commands for URD-6 goniometer with explanations and using examples :



We can set any measurement !

Theta Angle Correction

• THC s - set THeta angle Correction = shift Theta value per 's' degrees

Device working mode setting

- MOD 1 set Theta angle only scan MODe (2Theta angle = constans)
- MOD 2 set 2Theta angle only scan MODe (Theta angle = constans)
- MOD 3 set Theta & 2Theta angles simultaneously moving scan MODe

Work parameters setting

- INT t set counting time (INTerval) per 't' seconds
- STP p at MOD 1 set STeP scan Theta angle per 'p' value - at MOD 2 and MOD 3 - set step scan 2Theta angle per 'p' value

Angles setting

- STH a Set THeta angle per 'a' value (2Theta angle not moving)
- STT a SeT 2Theta angle per 'a' value (Theta angle not moving)
- SAN a Set 2theta ANgle per 'a' value, set Theta angle per 'a/2' value

Scanning

• SSC r - Start SCanning with a given step (STP) Theta angle only (MOD 1) either 2Theta angle only (MOD 2) either simultaneously Theta & 2Theta angles (MOD 3) from the current position (STH, STT, SAN) by 'r' degrees distance

Using examples :

The diffraction measurement within 3 angle's ranges, with difference steps, with the time interval = 5 s

	MOD 3 INT 5	 simultaneously scanning of 2Theta & Theta angles counting time = 5 seconds
•	SAN 23 STP 0.05 SSC 10	 set 2Theta angle = 23° & Theta angle = 11.5° set 2Theta angle step for scanning = 0.05° make a step scan from current position for a 10°
•	SAN 44.5 STP 0.02 SSC 2	 set 2Theta angle = 44.5° & Theta angle = 22.25° set 2Theta angle step for scanning = 0.02° make a step scan from current position for a 2°
• •	SAN 90 STP 0.1 SSC 20	 set 2Theta angle = 90° & Theta angle = 45° set 2Theta angle step for scanning = 0.1° make a step scan from current position for a 20°

The diffraction measurement within 2 angles ranges, with the same steps and with the time interval = 2.5 s

•	MOD	3	- simultaneously scanning of 2Theta & Theta angles
•	INT	2.5	- counting time = 2.5 sec
•	STP	0.04	- set 2Theta angle step for scanning = 0.04°
	SAN SSC		 set 2Theta angle = 25° & Theta angle = 12.5° make a step scan from current position for a 10°
•	SAN	50	

• SSC 1.5

The diffraction measurement within 1 angles range, with a shift of Theta angle

- MOD 3 simultaneously scanning of 2Theta & Theta angles
- INT 5 counting time = 5 sec
- SAN 30 set 2Theta angle = 30° & Theta angle = 15°
- STH 14 set Theta angle = 14°
- STP 0.05 set 2Theta angle step for scanning = 0.05°
- SSC 2 make a step scan from current position for a 2°

The measurement with Theta moving only

	MOD	1	- Theta angle scanning only
•	MOD	T	e e .
•	INT	5	- counting time = $5 \sec$
•	SAN	30	- set 2Theta angle = 30° & Theta angle = 15°
•	STH	14	- set Theta angle = 14°
•	STP	0.05	- set Theta angle step for scanning = 0.05°
•	SSC	2	- make a step scan from current position for a 2°

The measurement with 2Theta moving only

- MOD 2 2Theta angle scanning only
 INT 5 set counting time = 5 sec
 SAN 26 set 2Theta angle = 26° & Theta angle = 13°
- STT 25 set 2Theta angle = 25°
- STP 0.05 set **2Theta** angle step for scanning = 0.05°
- SSC 2 make a step scan from current position for a 2°

The short description of the software and hardware for URD-6 diffractometer steering

How to begin the work?

- 1. Turn on the computer
- 2. Start the URD-6 software
- 3. Turn on the CAMAC crate
- 4. Turn on the DRONEK-3. This text will appear inside the URD-6 software window :

URD-6 GONIOMETER CONTROLLER ver. October 2007 by Waclaw Musial "ELEKTRONIKA JADROWA" tel. +48 12 266-94-74 ul. Kobierzynska 93/43 30-382 Krakow Poland C=

5. Press ENTER key. This text will appear inside the URD-6 software window :

2THETA	:	not synchronized
THETA	:	not synchronized
MOD	:	3
INT	:	1.00
STP	:	0.0500
TH Corr	:	0.0000

- 6. Set the radiation detector high voltage supply. The HV Power Supply type 1904 have a special protection, so after the main power switch on you have to set the null (0) output voltage before you set any other HV value. Check if the red LED marked "OUTPUT" is shining.
- 7. Turn on the RTG tube power supply
- 8. Make the synchronization of the goniometer's axes passing up through the 4.5° positions :
 - choose the Hardware / Status menu option. The Status command begins sending continuously to the Dronek
 - using the switches on the Dronogur CAMAC block move the goniometer's axes down to the 2Theta/Theta = circa $4^{\circ}/2^{\circ}$
 - using the 2Th switch move the 2Theta axis fast up for circa 2 seconds (to the 6° position)
 - using the Th switch move the Theta axis fast up for circa 4 seconds (to the 6° position)
 - Check the message from the Dronek. It should be like : us

С

C =

2THETA	:	6.9260
THETA	:	6.5345
MOD	:	3
INT	:	1.00
STP	:	0.0500
TH Corr	:	0.0000
=		

- Close the URD-6 Status window
- choose the Hardware / Send TH Corr. menu option. The THC command with the adequate parameter sends to the Dronek

How to go on the work?

- 9. Prepare the sample and fit it on the sample holder
- 10. Prepare the command file to carry out the measurement
- 11. Choose the Measurement / Commands / Load menu option and select the proper file. Next you can correct the measurement algorithm choosing the Measurement / Commands / Edit menu option
- 12. Open the X-ray shutter
- 13. Choose the <u>Measurement / Run</u> menu option
- 14. You can also make a measurement directly typing the commands on the keyboard
- 15. Check the proper run of the measurement looking at the goniometer and the URD-6 software windows (text and diagram). If there is any improper command at the command file (bad syntax or parameter out of range), the measurement breaks
- 16. You can break the measurement at any time choosing the *Measurement / Break* menu option

- 17. The measurement's data are drawing on line. You can select a lot of manners of drawing it:
 - 2Theta, Theta or Point Number at the horizontal scale
 <u>View / F(2Theta)</u>
 <u>View / F(Theta)</u>
 <u>View / F(Point)</u>
 - linear or logarithmic vertical scale $\underline{View}/Log/Lin$ Ctrl+GThe logarythmic vertical scale is very useful to represent a small and a high peaks together



Illustration 1 Logarythmic Y scale

- with or without the background cutting

<u>View / Background</u> Ctrl+B

You can also switch on/off the movable marker to easy assign the digital values to the diagram point. $\underline{View} / \underline{Scan}$

- 18. You can magnify the fragment of the diagram :
 - <u>View / Scan</u> the movable marker appears on the diagram. You can check every data point for the point's number, 2Theta angle, Theta angle, interplanar distance (d), intensity. Move the thumb tab of the scroll bar to change the marker position



Illustration 2 The whole data diagram with the movable marker

The marker's position determines the centre of the zooming sector. Now you can manipulate with zooming :

– <u>V</u> iew / Zoom <u>I</u> n	Ctrl + I	the sector grows big twice
– <u>V</u> iew / Zoom <u>O</u> ut	Ctrl + O	the sector grows smaller twice







Illustration 4 Zoom 4X

- <u>V</u>iew / Zoom <u>C</u>enter

Ctrl + C the sector shifts to place the marker is in the center of the diagram



Illustration 5 The marker's position before Zoom Center



Illustration 6 The marker's position after Zoom Center

- <u>*View* / <u>*Zoom*</u> AutoScale Ctrl + Y - the vertical scale is stretched automatically in every sector</u>



Illustration 7 The zoomed and automatically stretched sector

- <u>View / Zoom All</u> Ctrl + A the whole data are drawing
- 19. After the commands file executing is finished the computer beeps for a 3 times
- 20. During the measurement or after it is complete you can save the results choosing the *File / Save* <u>As</u> menu option. There are two data formats at choice:

/Diffraction : only 2Theta positions + counts for a simple diffraction measurement (2Th = 2*Th)

Data from URD-6 diffractometer 28-09-2007 12:23:53 Lampa Cu 6 2.50 'Number of data, Time of counting [s] 60.000 342 1693 60.050 18752 60.100 60.150 18485 60.200 1763 342 60.250

/*Full Data* : 2Theta and Theta positions + counts for a complex measurement (2Th <> 2*Th)

Data from URD-6 diffractometer 28-09-2007 12:24:32 Lampa Cu 6 2.50 'Number of data, Time of counting [s] 60.000 30.000 342 60.050 30.025 1693

60.100	30.050	18752
60.150	30.075	18485
60.200	30.100	1763
60.250	30.125	342

Be careful : you lose your complex measurement's data, if you save it in the simple *Diffraction* format !

Remember : There is the interval time information in the DataFile. To ensure the proper recognition of the set up interval time in the Dronek device you have to enter the INT or the STATUS command at least one time per session.

21. You can switch on or off the Data File Autosaving clicking on the *File / AutoSaving* menu At every new data point the data file will be updated.

22. You can have a look at the data file choosing the *File / List Data* menu option

How to make the next measurement?

- 23. Save the old measurement data
- 24. Close the X-ray shutter
- 25. Choose the <u>Measurement / New</u> menu option and confirm it.
- 26. Enter the title for the new measurement
- 27. Select the new command file
- 28. Prepare the sample and fit it on the sample holder
- 29. Continue from the 12 item of this instruction

How to finished the work?

- 30. Close the X-ray shutter
- 31. Save the last measurement data
- 32. Choose the <u>*File / Exit*</u> menu option and confirm it

The SAN 4 command will be automatically send to the goniometer controller. It is for the future to facilitate the goniometer's axes synchronisation and the sample fitting

33. Set the null (0) output voltage for the radiation detector (also for the future - see item 6)

How to install the URD-6 software ?

- 1. Create the new directory on the hard disk named \URD-6
- 2. Create the subdirectory \URD-6\DATA
- 3. Copy the files : URD6.EXE and MANUAL_URD6.PDF to the \URD-6 directory
- 4. Create the shortcut on the desktop to the URD6.EXE
- 5. Click on the shortcut by right mouse button
- 6. Set the Properties / Working Directory to \URD-6\DATA
- 7. Click on the shortcut by left mouse button
- 8. Choose the *Hardware / Config* menu option

Hardware Configu	ration		
Enter password :			
****			ОК
COM port	X-ray Tube	Theta Corr.	
COM2 -	Cu 🔻	0.013	Cancel
· _		,	

- 9. Select the proper COM port
- 10.Select the proper X-ray tube
- 11.Enter the Theta Correction value. Note : this value **adds** to the current Theta Angle value to reduce the Theta Synchronization Error to nil.
- But you have to use the *Hardware / Send TH Corr*. menu option to send this value to Dronek 12. Enter the current password
- 13. The password is the 4-digit number calculated on the following manner :
- $Password = day + month + year \quad \text{for example: } 30 + 08 + 2007 = \underline{2045}$

14. Click OK button

How to get the better URD-6 software ?



Simply write an e-mail to me with detailed description of your problems. I will try to find a remedy and I will send you the new version of the URD-6.EXE file

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