# XAS software

To run a XAFS spectrum you need to use the scan control program. See below:

📼 Scan Cont	trol - 1								X	
Eramework Ge	eneral <u>S</u> can <u>M</u> isce	llanoeus <u>T</u> ools	;							
	Scan Contr	ol - SR12	ID01H	<b>U02IO</b>	C01:sca	n1		- ? 5	ď	
sca	n1	scan2	8	can3		scan4	an4 scanH			
Sync	Clear Apply	Start	Pause	Go	Abort	Plot	Referenc	e Refresh		
General Phase		Busy		Pause	Data Read	ly Data:	State	Alert		
IDLE		Not Bus	y	GO	Yes	POS	TED	No	4	
Status	SCAN Complete	B				Max F	Points	Num Points		
Data	Wrote data to	o SR12ID01	H0569.n	ıda		-	2048	539		
Directory	/beamline/da	ta/user_da	ta/2009	9/1/960				539		
Positioner(s)				Detectors						
Primary				1						
Set Point			•	2						
Read Back				3					_	
Secondaru				4						
Set Point				5						
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Triggers				8						
Trigger 1				9						
Trigger 2			1	0						
Trigger 3			1	1						
Trigger 4			1	2					-	
<ul> <li>Simple Scan</li> </ul>	1									
5	Start		End	S	tep-Size	Tir	ne	Num Points		
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You will also need the XAFS endstation GUI to do basic operations before running the spectrum: centre the sample, upload the right positions for the sample holder and adjust the gains of the keithleys.



You can find these interfaces, already opened, in the pc, labelled PC1.

To acquire correctly the spectrum you need to follow these steps:

### • Centre your sample

- $\circ$  Go to the scan control program.
- Left-click on 'positioner(s) Primary'

📼 Scan Cont	rol - 1								×		
<u>F</u> ramework <u>G</u> e	eneral <u>S</u> car	n <u>M</u> iscellar	noeus <u>T</u> ool	s							
	Scan	Control	l - SR12	ID01H	<b>HU02IO</b>	C01:scar	11		- ? 🕁 💕		
sca	n1	sc	an2		scan3	50	can4	an4 scanH			
Sync	Clear	Apply	Start	Pause	Go	Abort	Plot	Referen	ce Refresh		
General —											
Phase			Busy		Pause	Data Ready	Data	State	Alert		
IDLE			Not Bu	sy	GO	Yes	POS	TED	No		
Status	SCAN Co	mplete					Maxi	Points	Num Points		
Data	Wrote d	lata to	SR12ID01	H0569.	mda			2048	539		
Directory	/beamli	ne/data	/user_da	ta/200	9/1/960				539		
Positioner(s)					Detectors						
Primary	None		•		1				<b>—</b> • <b>—</b>		
Set Point	None			•	2						
Read Back	Energy Table	Ý		0	3						
Secondary	RT hol	der Y			4						
Set Point	Cryost	der X tage X	-	10	5						
Read Back	Cryost	tage Y	r v	ic	6						
	Rotary	Stage			7						
Triggers -	BPM D DAC1	ACout			8						
Trigger 1	JJ Slits	V centre			9						
Trigger 2	JJ Slits JJ Vert	T Centre			10						
Trigger 3	JJ Hori	z I			11						
Trigger 4	LINDSL	Centre			12				🗌 <sup>©</sup> 💂		
📄 Simple Scan											
5		Start		End	9	Step-Size	Ti	ime	Num Points		
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								/Time Pro	ofiles		
12								03	Mar 09 11:29:23		

Select: RT holder (x and y) if you are performing measurements at room temperature; Cryostage (x and y) if you are measuring at cryotemperature.

 $\circ$   $\;$  Left click on Detectors.

🔤 Scan Cont	trol - 1									×	
<u>F</u> ramework <u>G</u> e	eneral <u>S</u> car	n <u>M</u> iscellan	oeus <u>T</u> ools								
	Scan (	Control	- SR12	ID01H	IU02IO	C01:scar	11		- ? 5	ď	
sca	in1	SCa	in2		scan3 sca			n4 scanH			
Sync	Clear	Apply	Start	Pause	Go	Abort	Plot	Referenc	e Refresh		
General Phase IDLE Status Data	SCAN Co Wrote d	mplete ata to :	Busy Not Bus SR12ID01	у H0569.	Pause GO mda	Data Ready Yes	Data POS Max F	State TED Points 2048	Alert No Num Points 539		
Positioner(s) Primary Set Point Read Back Secondary Set Point Read Back	RT h	older Y 01.00000 00.99987		•	Detectors	8					
Triggers Trigger 1 Trigger 2 Trigger 3 Trigger 4					Read Tin 8 Crystal 9 UHV BPI 10 UHV BPI 11 ION BPN 12 ION BPN	me Temperature rrent M Intensity M Y position M X position M Y position I Intensity	e				
Simple Scar	1(	Start 0 . 00000	20.	End 00000	SI O .	ep-Size 10000	Tii 1.00 RT ho	me D <b>000</b> older Y/Tim	Num Points 101 ne Profiles	;	
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For scanning the positions you need I0, I1, I2, which are related to the incoming beam, the flux after the sample, and the flux after the reference, respectively.

• Enter the min and max values and the steps into the 'simple scan' region at the bottom of the window.

Scan Cont	r <mark>ol - 1</mark> neral Scar	n Miscellar	neus Too	ls							
<u></u>	Scan	Control	- SR12	2 <b>ID</b> 0	1HU	0210	C01:sca	n1		- <mark>?</mark> 5	
sca	n1	sca	an2		sca	n3		scan4		scanH	
Sync	Clear	Apply	Start	Pau	use	Go	Abort	Plot	Referen	ce Refresh	
General											
Phase			Busy		Pa	use	Data Rea	dy C	)ata State	Alert	
IDLE			Not Bu	sy	G	9	Yes		POSTED	No	
Status	SCAN Co	mplete						N	/lax Points	Num Points	
Data	Wrote d	lata to	SR12ID0	1H056	9.md	a		_	2048	539	
Directory	/beamli	ne/data	/user_d	ata/2	009/	1/960				539	
Positioner(s)					Del	tectors -					
Primary	RT h	older Y			1	Angle	e	()	16.20837	deg 🔽 🔿	
Set Point	1	01.00000	) mm 📕	•	2 Energy				7.08283	keV 🚺 🔿	
Read Back	1	00.99987	7 mm 📃	0	3	3 Time			5018	5270 📕 🔿	
Secondary					4	IO			60	0922 📃 🔿	
Set Point			Г	10	5	I1			10	6874 📃 🔿	
Read Back			Ē	iol	6	12			70:	2500 🔲 🔿	
					7						
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Trigger 1		I	Done	-	9						
Trigger 2				-	10						
Trigger 5				-	11						
ringger 4			L		12						
Simple Scan											
5		Start		End		S	tep-Size		Time	Num Points	
	9	0.00000	110	.0000	00	0	.50000	1	.00000	41	
								R	T holder Y/Ti	me Profiles	
the state											

• **Apply** the scan parameters and start the scan. Please notice that your values must be **applied** before starting the scan. The plot window should pop up automatically. If it does not, press the plot button. To visualise the plot correctly you **must** select on the scan control program the variable that you want as the x variable (In this case the position of the sample holder).

sca	1 9	can2	scan3	scan	4	haree	
) sca			soano		·	scann	
Sync	Clear Apply	Start Par	ise Go	Abort	Plot Refere	ence Refresh	
General							
Phase		Busy	Pause	Data Ready	Data State	Alert	
IDLE		Not Busy	GO	Yes	POSTED	No	
Status			A CONTRACTOR		Max Points	Num Points	
Data	Wrote data to	SR12ID01H056	9.mda		2048	4:	
Directory	/beamline/data	a/user_data/2	009/1/960			539	
Positioner(s)			Detectors				
Primary	RT holder	Y O	1 Angle		16.2083	7 deg 0	
Set Point	101.0000	0 mm	2 Energ	у	7.0828	3 keV	
Read Back	100.9998	7 mm	3 Time		501	85270 🔲 🔿	
Secondary			4 10			60922 🔲 🔿	
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Read Back			6 12		70	02500	
The <b>w</b> to see an		_	7				
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Trigger 1		Done	9				
Trigger 2			10				
Trigger 3			11				
Trigger 4			12				
Simple Scan							
5	Start	End	St	ep-Size	Time	Num Point	
	90.00000	110.000	0.00	50000	1.00000	4	
					D.T. 1.1. 1.1.	Time De Class	

You have also to select in the plot window which variable you want to see as the y variable.

• Once you have identified the x and y centre for your samples (and your references) you have to upload these values. To do that select 'Sample pos' and 'reference pos' from the endstation GUI.







## • Click on 'more':

X positi	ionXY.adl			_ <b>— X</b>
Sample				
$\square$	Colored	X Position	Y Position	Description
	Select	p+000	p+000	<u>ا</u> ـــــا
$ \bigcirc $	Select	0.000	0.000	ļ
$ \bigcirc$	Select	0.000	134,000	Sample 5
	Select	0.000	114,000	Sample 4
$ \bigcirc $	Select	0.000	94,000	Sample 3
$ \bigcirc $	Select	0.000	74.000	Şample 2
	Select	0.000	54.000	Şample 1
也Motors				
	Y			

• Enter the correct values for the x and y of the different samples. To centre each sample it is now sufficient to click on the respective 'select' button.

### • Verify that the gains of the keithleys are set correctly.

To do that you need first to check that the signals for I0, I1 and I2 are within 1 and 10. These values are displayed in the upper side of the electronic rack near Hutch B. They are labelled as I0, I1 and I2.



You should adjust the keithley (Keithley1, Keithley2 and Keithley3 for I0,I1 and I2, respectively) gains in order for these values to be in the right range. Click on the keithley button in the endstation GUI



The following window will pop up:



Select the right value from the gain button.

### • Run the EXAFS scan

- $\circ$  Go to the scan control program.
- Left-click on 'positioner(s) Primary'

🔤 Scan Control - 1	×
<u>F</u> ramework <u>G</u> eneral <u>S</u> can <u>M</u> iscellanoeus <u>T</u> ools	
Scan Control - SR12ID01HU02IOC	01:scan1 ? 🔁 🗃
scan1 scan2 scan3	scan4 scanH
Sync Clear Apply Start Pause Go	Abort Plot Reference Refresh
General	
Phase Busy Pause	Data Ready Data State Alert
IDLE Not Busy GO	Yes POSTED No
Status SCAN Complete	Max Points Num Points
Data Wrote data to SR12ID01H0569.mda	2048 539
Directory /beamline/data/user_data/2009/1/960	539
Positioner(s) Detectors	
Primary None 1	<b>—</b> • <b>•</b>
Set Point None 2	
Read Back Table V C 3	
RT holder Y 4	
Set Point Cryostage X D C 5	
Bread Back Deformance halden Y	
Rotary Stage 7	<b>—</b>
Triggers BPM DACout 8	
Trigger 1 JJ Slits V centre 9	
Trigger 2 JJ Slits H centre 10 10	
Trigger 3 JJ Horiz I 11	
Trigger 4 MIDSLY Centre 12	
Simple Scan	
🕤 🕤 Start End Ste	p-Size Time Num Points
10.00000 20.00000 0.3	10000 1.00000 101
	/Time Profiles
10 A	03 Mar 09 11:29:23

- Select Energy
- $\circ$  Left click on Detectors.
- Select: Angle, Energy, Time, I0, I1, I2

🔤 Scan Con	trol - 1								×
<u>Framework</u> <u>G</u> e	eneral <u>S</u> can <u>M</u> iscelland	oeus <u>T</u> ools							
	Scan Control	- SR12ID0	1HU	02100	C01:sca	an1		- ? 5	r
sca	in1 sca	n2	scar	13	1	scan4	1	scanH	
Sync	Clear Apply	Start Pau	se	Go	Abort	Plot	Referenc	e Refresh	
General —			2			19 - 12 - 18	-		
Phase		Busy	Pa	use	Data Rea	dy Data	State	Alert	
IDLE		Not Busy	G	0	Yes	POS	STED	NO	
Disto	Nucha Jaka ka f		Max	Points	Num Points				
Directoru	wrote data to s	neer data /2	9.maa	1 /960			2040	530	
=	/beamine/data/	user_uata/2	-	., 500				555	
Positioner(s)			Det	ectors					
Primary	Energy		1	Angle		16	20838	deg 📃 🖸	
Set Point	7.08	975	2	2 Energy			7.08283 keV		
неад васк	7.08977 (k	ev)	3	Time			50185	270	-
Secondary			4	10			60	922 🗌 🖸	
Set Point			5	11			106	874	
Read Back			6	12			702	500	
– Triggers –			7						
Triggers	D	one 🗖	8						
Trigger 2			10						
Trigger 3			11						
Trigger 4			12						
E Simple Scar	1								
	' Start	End		SH	an-Siza	т	ime	Num Points	
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						<b>F</b>		Profiles	
					_	En	ergy/11me1	Fromes	1
AI	oply complete						03 M	4ar 09 16:16:34	

• To set the EXAFS scan parameters go to 'EXAFS Scan' section by clicking on the arrow on the left bottom of the window.

– Simple Scan –
5

This button allows switch between 'simple scan' and 'EXAFS scan mode'.

Select the element and the edge (K or L3) that you want to measure by clicking on the 'Element(K)' or 'Element(L3)' button. A periodic table window will pop up. Click on the desired element.

riodic	: Table																	
н						Bi 83	3 Bis	muth										He
Li	Be												В	С	N	0	F	Ne
Na	Mg												AL	Si	Р	S	CI	Ar
К	Ca		Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr		Y	Zr	NЬ	Мо	Tc	Ru	Bh	Pd	Ag	Cd	In	Sn	Sb	Te	1	Xe
Cs	Ba		Lu	Hf	Ta	W	Re	Os	lr	Pt	Au	Hg	TI	РЬ	Bi	Po	At	Rn
Fr	Ra	**	Lr	Rf	DЬ	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo
* La	inthano	ids	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	ТЬ	Dy	Ho	Er	Tm	ΥЬ		
** Ac	ctinoids		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	С	ancel

This upload the values suited for the selected edge: the edge energy, the energy intervals, the energy steps and the integration time. The number of points in each interval (Num Points) and the number of points in total (Total Points) are calculated on the basis on the given parameters. If you are not satisfied with the given parameters you can change them by inserting a new value. In the pre-edge and edge ranges (phase 1 and 2) the step-size is given in eV (energy space) whereas in phase 3 is given in Å<sup>-1</sup> (K space). Usually you may want to increase the energy resolution in the edge region. Minimum resolution values vary with energy and monochromator crystals. Typical values are around 0.25 eV. For the integration time you have the possibility to choose between two 'time modes': square and linear. This will simply change the function through which the integration time is increasing.

You have to press the 'apply' button in order to upload the scan record. When the selected values are actually uploaded the colour of the squares should change from red to green.

• Press start to begin the scan. The plot window should pop up automatically. If it does not, press the plot button.