## MiniFlex 600

- 1. Sign the log sheet. When finished be sure to enter the total time in decimal hours.
- 2. Log onto the control computer using your NetID /password.
- 3. Turn on the diffractometer. Press the **On** button then the Door access button to stop the beeping sound.



- 1 Door access. When flashing and beeping door is unlocked.
- 2 Indicator light
- 3 Enable/Disable key. When key is removed diffractometer is disabled
- 4 Off button
- 5 On button
- 6 Emergency Stop Button

4. Start the control program. Double click MiniFlex Guidance on the desktop. The MinFlex Guidance login screen will appear with your NetID as the default Login name. Click OK. The MiniFlex *Starting* window will appear as the system initializes.



# 5. Once the system has initialized the main window will open.

🚳 MiniFlex Guida	nce - kjbalo	lwin(Sy	stem Manage
File Edit Tasks	View C	ontrol	Options V
Hardware Status		ά×	
E II			
ltem	Status	C	
🔄 Theta/2-Theta	10.000 de	g O	
🔚 XG power	On	-	
XG_error_code	0	-	
🚼 X-ray	Off	-	
🚼 Target	Cu(Ka)	-	
🕜 Tube voltage	-	-	
🕜 Tube current	-	-	
- Shutter	Close	-	
🛞 Water flow	0.0 L/min	-	
Detector	Main Dete	e	
🗐 Data acquisiti	-	-	
<del>=</del> HV # 1		-	
🗐 PHA baseline	38 div	-	
PHA window	14 div	-	
Count mode	Differentia	al -	
Angle correcti	Disable	-	
Angle correcti	-	-	
Slit correction	Disable	-	
🚭 Soller(inc.)	5.0deg	-	
会 i HS	10.0mm	-	
€DS	1.250deg	-	
eess	8.0mm	-	
Soller(rec.)	5.0deg	-	
€ RS	13.0mm	-	
🖶 Filter	K-beta(x2	) -	
🕀 Monochroma	None	-	

## 6. Select Tasks → Package/Macro Management and View → Package Bar



MiniFlex Guidance - kjbaldwin(System Manager)											
File Edit Tasks	View Control Options Window Help										
Hardware Status	✓ <u>H</u> ardware Status History										
Item Theta/2-Theta XG power	Package bar <u>F</u> low Bar										
☑ XG_error_code ☑ X-ray ☑ Target ☑ Tube voltage	Initialize <u>L</u> ayout <u>P</u> rofile Window Setup Window Style										
☑ Tube current ➡ Shutter	 Close -										

7. When the Package window opens double click General Measurement



If you exit the program correctly, steps 6 and 7 will be remembered and will not have to be repeated the next time you run *MiniFlex Guidance*. 8. The *Package/Macro Measurement* window will open.

Package/Macro Measurement	×
General Measurement	<ul> <li>✓ Open</li> </ul>
New Package Bar	Save As
Duplicate 🔺 💙 Delete	Group ?
General Measuremer	nt
Startup	Execute
1 General Measurement	

9. Turning on the x-ray generator. Turn on the Haskris heat exchanger then click Startup in the *Package/Macro Measurement* window.



10. The generator *Startup* window will open. Leave *Generator usage:* as *Use everyday* and click *Execute*. The *Turning On X-ray Generator* message will popup followed by *Aging process started*. This will take a few minutes.





Ĩ	Hardware C	Control		stem
	Status:	Remaining	00:00:22	Opt
<b>A=</b> 0	Aging proce	ess started.	^	
				Pa
			X	G
			Abort	
R	XG	_error_code 0	-	

11.When the generator is on and ready you can click *OK* in the *Startup* window then *1 General Measurement* in *Package/Macro Measurement* window

ALC: NO	🞯 MiniFlex Guida	nce - kjbaldwin(Sy	tem Manager)
1	File Edit Tasks	View Control	Options Window Help
le	Hardware Status	џ×	
	E B		Package/Macro Measurement ×
1000	Item	Status C	General Measurement V Open
100 LUIS	🔄 Theta/2-Theta	10.000 deg 0	New Package Bar Save As
al	XG power	On -	Duplicate A V Delete Group ?
	XG_error_code	0 -	Startup X
	X-ray	On -	General Measurement Timer
	Tube welte en	Cu(Ka) -	Start     Start
	Tube voltage	40 KV -	Execute 8/13/2022 T 01:01:01
ob		Close	Shutdown
er	Water flow	3.51/min -	Esumated bE: 2022/08/13 01:04:24
		Main Dete	1 General Measurement Generator usage: Use everyday 🗸
	Data acquisiti		XG set: Hold 🗸
	HV # 1	-	
	PHA baseline	38 div -	Voltage(KV) : 20 Current(mA) : 2
	PHA window	14 div -	Even to OK Canad
	🔁 Count mode	Differential -	
	Angle correcti	Disable -	
4	Angle correcti		
	Slit correction	Disable -	
.h	Soller(inc.)	5.0deg -	
	IHS	10.0mm -	
	e DS	1.250deg -	
2	SS SS	8.0mm -	
9	Soller(rec.)	5.0deg -	
w	RS C	13.0mm -	
	Thilter	K-beta(x2) -	
	The second secon	None -	

## 12a *General Measurement* Check the first check box.

Genera	al Measurement									-			×
🗌 Au	utomatic generation o	f data file names											
No.	Exec. Folder		File name		Sample name	V	Memo	🗸 Condit	tion	Analysis condition	Spin	Sam	ple
1 (								No1	$\sim$	Set		1	
2								No1		Set		1	
3								No1	~	Set		1	$\sim$
4								No1		Set		1	
5								No1		Set		1	
5								No1		Set		1	
· ·								No1		Set		1	
0								No1		Set		1	
э 10				•••				No1		Set		1	
10								INOT		Set		1	
XG t	ermination condition		Show optical d	evices conf	irmation message								_
<b>О</b> Т	he status quo	) Stop the X-Bav	Show	🔿 Don't	show				Se	t Meas. Con	dition	S	
<u> </u>		· · · · · · · · · · · · · · · · · · ·	0	0								ſ	?
												L	
	Run								ок		С	ancel	

12b General Measurement continued. Click the navigation button..

Packag	ge Bar	Save	As												
Gener	al Me	asurement										-			×
	utoma.	itic generatio	n of data file i	names				_				Analysis			
No.	Exec	c. Folder			File name		Sample name		Memo	Conditi	ion	condition	Spin	Samp	ple
1							J			No1	~	Set		1	
2										No1		Set		1	
3										No1	~	Set		1	
4										No1	$\sim$	Set		1	
5										No1	~	Set		1	
6										No1	$\sim$	Set		1	
7										No1		Set		1	
8										No1		Set		1	
9										No1		Set		1	
10										No1		Set		1	
×G	termina	ation conditio	on		Show optical	devices coi	nfirmation message	I			6-4	Mars Car	Ja:		_
	The sta	atus quo	O Stop the	•X-Ray	Show	ODor	n't show				Set	meas. Con	ations		
															?
	Run										ок		Ca	ancel	

### 12c Navigate to mysbfiles and enter an appropriate filename and click Save



12d General Measurement continued. Sample name and Memo are text fields, enter any information you want or they may be left blank. Leave Condition as No1 and click Set Meas. Conditions...

Genera	l Me	asurement							_			×	Ma
□ Au	itoma	tic generation of data file names											Ge
No.	Exec	2. Folder 🛛 🔽	File name		Sample name	🚺 Memo	Condit	tion	Analysis condition	Spin	Sam	ple	Ba
1		X:\Rigaku\miniflex\Corundum\	Corundum-8-12-22.ras				No1	_~	Set		1		
2							No1		Set		1		
3							No1		Set		1		ts i
4							No1		Set		1		
5				•••			No1		Set		1		
5							No1		Set		1		
0							No1		Set		1		
0 9				•••			No1		Set		1		
10							NoI NoI		Set		1		
10				••••			NUT		Jet				
XG to	ermina	ation condition	Show optical devices	confin	mation message								
O T	he et:	atus quo 🔷 Stop the X-Bau	Show	Don't «	show			Set	Meas. Con	ditions			
	ne ste		g anon O	Donre							Γ	2	
											L	:	
	Run							ок		Ca	ancel		

#### 13a Measurement Condition

Olk	condition	า					Back	groun	d conditi	ion	
01	Variable	slit system		🖲 Vari	able+Fixed slit	system	Ba	ackgro	und mea	asurements	s
Opt	ical devi	ces									
	Soller(ii	nc.)	IH	S	D	S					
5.0	deg	$\sim$	10.0 mm	`	<ul> <li>1.250 deg</li> </ul>	, ~					
	SS		Soller(	rec.)	F	IS I	Monoch	romati	zation		
13.0	0 mm(0 p	n) 🗸	5.0 deg	`	<ul> <li>13.0 mm(0</li> </ul>	)pen) 🗸 N	lone		<b>*</b>		
Mea	asuremei	nt condition	1		Edit the meas	urement conditi	ons	Fil	e create		
Pres	set Cond	lition			Сору	Reset	t		Individu	ial configui	ration fi
N	lo1 N	o2 No3	No4 N	No5 N	lo6 No7	No8 No9	No10				
S	can axis	Theta	/2-Theta	~	Mode: Co	ntinuous	~	ι	Jnit:	CPS	~
	_										
	Exec	: Start (deg)	Stop (deg)	Step (deg)	Speed (deg/min)	Comment		Voltag (kV)	e Curren (mA)	t Backgri conditio	ound ons
		: Start (deg)	Stop (deg)	Step (deg)	Speed (deg/min)	Comment		Voltag (kV)	e Curren (mA)	t Backgri conditio	ound ons
<b>-</b> •(	Exec	:. Start (deg) 3.0000 3.0000	Stop (deg) 90.0000	Step (deg)	Speed (deg/min)	Comment		Voltag (kV) 40	e Curren (mA)	t Backgro conditio	ound ons
<b>-&gt;</b> (	Exec	2. Start (deg) 3.0000 3.0000 3.0000	Stop (deg) 90.0000 90.0000 90.0000	Step (deg) 0.02 0.02 0.02	Speed (deg/min)	Comment		Voltag (kV) 40 40	e Curren (mA) 15 15	t Backgru conditio Set Set	ound
-•(	Exec	2. Start (deg) 3.0000 3.0000 3.0000 3.0000	Stop (deg) 90.0000 90.0000 90.0000	Step (deg) 0.02 0.02 0.02 0.02	Speed (deg/min) 10.0 10.0 10.0 10.0	Comment		Voltag (kV) 40 40 40 40	e Curren (mA) 15 15 15 15	t Backgruconditio	ound
	Exec 1 2 3 4 5	2. Start (deg) 3.0000 3.0000 3.0000 3.0000 3.0000	Stop (deg)           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000	Step (deg) 0.02 0.02 0.02 0.02 0.02	Speed (deg/min) 10.0 10.0 10.0 10.0 10.0	Comment		Voltag (kV) 40 40 40 40 40	e Curren (mA) 15 15 15 15 15	t Backgruccondition	ound
-•(	Exec 1 2 3 4 5 6	2. Start (deg) 3.0000 3.0000 3.0000 3.0000 3.0000 3.0000	Stop (deg)           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000	Step (deg)           0.02           0.02           0.02           0.02           0.02           0.02	Speed (deg/min)           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0	Comment		Voltag (kV) 40 40 40 40 40 40 40	e Curren (mA) 15 15 15 15 15 15	t Backgruce conditions Set Set Set Set Set	ound
<b>_</b> ▶(	1 2 3 4 5 6 7	2. Start (deg) 3.0000 3.0000 3.0000 3.0000 3.0000 3.0000 3.0000	Stop (deg)           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000	Step (deg)           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02	Speed (deg/min)           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0	Comment		Voltag (kV) 40 40 40 40 40 40 40 40	e Curren (mA) 15 15 15 15 15 15 15 15 15	Backgruce condition Set Set Set Set Set Set Set	ound
-•(	Exec 1 2 3 4 5 6 7 8	<ul> <li>Start (deg)</li> <li>3.0000</li> <li>3.0000</li> <li>3.0000</li> <li>3.0000</li> <li>3.0000</li> <li>3.0000</li> <li>3.0000</li> <li>3.0000</li> <li>3.0000</li> </ul>	Stop (deg)           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000	Step (deg)           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02	Speed (deg/min)           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0	Comment		Voltag (kV) 40 40 40 40 40 40 40 40 40	e Curren (mA) 15 15 15 15 15 15 15 15 15 15	t Backgruce conditions Set Set Set Set Set Set Set Set	ound
	Exect 1 2 3 4 5 6 7 8 9	2. Start (deg) 3.0000 3.0000 3.0000 3.0000 3.0000 3.0000 3.0000 3.0000 3.0000	Stop (deg)           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000	Step (deg)           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02	Speed (deg/min)           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0	Comment		Voltag (kV) 40 40 40 40 40 40 40 40 40 40	e Curren (mA) 15 15 15 15 15 15 15 15 15 15 15	t Backgruce condition Set Set Set Set Set Set Set Set Set	ound
_ <b>-</b> •(	Exect 1 2 3 4 5 6 7 8 9 10	<ul> <li>Start (deg)</li> <li>3.0000</li> </ul>	Stop (deg)           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000	Step (deg)           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02           0.02	Speed (deg/min)           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0	Comment		Voltag (KV) 40 40 40 40 40 40 40 40 40 40 40	e Curren (mA) 15 15 15 15 15 15 15 15 15 15 15 15	t Backgruce condition Set Set Set Set Set Set Set Set Set Set	ound
_ <b>→〔</b>	Exec 1 2 3 4 5 6 7 8 9 10 Calculate	<ul> <li>Start (deg)</li> <li>3.0000</li> <li>a.0000</li> <li>a.0000<!--</td--><td>Stop (deg)           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000</td><td>Step (deg) 0.02 0.02 0.02 0.02 0.02 0.02 0.02 0.0</td><td>Speed (deg/min)           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0</td><td>Comment</td><td></td><td>Voltag (kV) 40 40 40 40 40 40 40 40 40 40 40 40</td><td>e Curren (mA) 15 15 15 15 15 15 15 15 15 15 15</td><td>t Backgruce condition Set Set Set Set Set Set Set Set Set</td><td></td></li></ul>	Stop (deg)           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000           90.0000	Step (deg) 0.02 0.02 0.02 0.02 0.02 0.02 0.02 0.0	Speed (deg/min)           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0           10.0	Comment		Voltag (kV) 40 40 40 40 40 40 40 40 40 40 40 40	e Curren (mA) 15 15 15 15 15 15 15 15 15 15 15	t Backgruce condition Set Set Set Set Set Set Set Set Set	

Make the following changes so this information matches the physical setup of the diffractometer.

## Change *Monochromatization* to *kb filter (x2)*

Change SS to 8.0 mm

If you exit the program correctly, these changes will be remembered and will not have to be repeated the next time you run *MiniFlex Guidance*.

Check *box 1* and enter appropriate values for *Start Stop* and *Speed*. Leave *Step* as 0.02 13b Measurement Condition continued. Click *OK* and *General Measurement* panel will open. But first load the sample.

leasurement	Conditio	n								×	
Slit condition	1					Ba	ckgroun	d conditio	on		
🔘 Variable s	lit system		🖲 Varial	ble+Fixed slit :	system	E	Backgro	und mea:	surements		
Optical devic	es										
Soller(in	ic.)	IHS	5	D	s						
5.0 deg	$\sim$	10.0 mm	~	1.250 deg	~						
SS		Soller(	rec.)	R	s	Monoc	:hromati:	zation			
8.0 mm	~	5.0 deg	~	13.0 mm(C	lpen) 🗸	kb filter	(x2)	~			
Measurement condition Edit the measurement conditions File create diti											
Preset Condition     Copy     Reset     Individual configuration files       et.											
No1 No Scan axis:	D2 No3	No4 N	105 No	10de: Col	No8 No9 ntinuous	No10	ι	Jnit:	CPS	~	
Exec.	Start (deg)	Stop (deg)	Step (deg)	Speed (deg/min)	Comme	ent	Voltag (kV)	e Current (mA)	Backgrou condition:	nd	
1 🗹	15.000	95.000	0.02	40.0			40	15	Set	^	
2 🗌	3.0000	90.0000	0.02	10.0			40	15	Set		
3 🗌	3.0000	90.0000	0.02	10.0			40	15	Set		
4 🗌	3.0000	90.0000	0.02	10.0			40	15	Set		
5 🗌	3.0000	90.0000	0.02	10.0			40	15	Set		
6 🗆	3.0000	90.0000	0.02	10.0			40	15	Set		
7 🗆	3.0000	90.0000	0.02	10.0			40	15	Set		
8 🗆	3.0000	90.0000	0.02	10.0			40	15	Set		
9 🗆	3.0000	90.0000	0.02	10.0			40	15	Set		
10 🗌	3.0000	90.0000	0.02	10.0			40	15	Set	<b>v</b>	
Calculate	d scan dur	ation: 00:02	:27								
						(		ж		Canaal	

## 14 Load the sample.





14 General Measurement Click Run. A confirmation Message will pop up. Verify the information and click OK

Ge	nera	l Me	asurement							_			Packa
c [	] Au	itoma	tic generation of data file names										
	No.	Exec	. Folder 🛛 🔽	File name		Sample name 🛛 🚺	Memo 🚺	Conditi	on	Analysis condition	Spin	Sam	nple
	1	$\checkmark$	X:\Rigaku\miniflex\Corundum\	Corundum-8-12-22.ras				No1	~	Set		1	$\sim$
	2							No1		Set		1	
e	3							No1		Set		1	$\sim$
	4			1				No1		Set		1	~
	5							No1		Set		1	~
	5							No1		Set		1	~
	/ 0							No1		Set		1	~
	0 0							No1		Set		1	~
	3 10							No1		Set		1	
								NUT		Set			· ·
	KG te	ermina	ation condition	Show optical devices	s con	firmation message							
(	) TI	he sta	atus guo 🛛 Stop the X-Ray	🖲 Show 🛛 🔾	Don'	t show			Se	t Meas. Con	ditions	)	
		_											?
(		Run							ОК		C	ancel	



## 15 Data Collection in progress.



#### 16a Data Collection finished. Notice that *Theta/2-Theta* is back to the home position, 10.000 deg.



16b Data Collection finished. Open windows explorer and navigate to your *data directory*. Notice that three files have been created. *Corundum-8-12-22.ras* is file containing the raw data.

📙 🛛 🛃 🚽 🛛 Corundum				
File Home Share View				
← → ֊ ↑ 📙 < kjbaldwin (\\mysbf	iles.campus.stonybrook.edu) (X:) > Rigaku >	miniflex > Corundum	5 V	🔎 Search Corundum
FirefoxPortable	Name	Date modified	Туре	Size
IntelFortran	🖳 Corundum-8-12-22_Theta_2-Theta.asc	8/12/2022 10:31 AM	Ascii data	22 KB
Inventor Server for AutoCAD 2	Corundum 8 12 22_Theta_2-Theta.raw	8/12/2022 10:31 AM	RAW File	19 KB
KMS	Corundum-8-12-22.ras	8/12/2022 10:31 AM	RAS File	93 KB
LabVIEW Data	Corundum-3-31-22.ras	3/31/2022 11:10 AM	RAS File	105 KB
Match!	🖳 Corundum-3-31-22_Theta_2-Theta.asc	3/31/2022 11:10 AM	Ascii data	26 KB
MATLAB	Corundum-3-31-22_Theta_2-Theta.raw	3/31/2022 11:10 AM	RAW File	21 KB
👌 Music				
E Pictures				
Python3				

17a Adjusting the PHA to minimize Fe fluorescence. Adjust the PHA baseline and PHA window: Select *Options*  $\rightarrow$ *Detector Setup*  $\rightarrow$  1 *D/teX Ultra*. Enter the desired values and click *Register* 

	MiniFlau Cuida	n an Itila Ishain (Ca	atom Monore		~							
	WiniFlex Guida	nce - kjbaldwin(Sy	/stem Manage		🥶 MiniFlex Guida	nce - kjbaldwin(Sys	tem Manager) ·	[Profile]				
R	File Edit Tasks	View Control	Options V		🕮 File Edit Ta	sks View Contr	ol Options	Window Hel	D			
	Hardware Status	φ×		le l								
	P I				Hardware Status	Ψ×	. Q ↔ 🖾 :	E E € E 609				
	ltem	Status 0			P. 8.		Theta/2-Theta			Mode	Baseline	Window
	ち Theta/2-Theta	10.000 deg 0			Itom				1	Normal	28	1/
	🔚 XG power	On -		-		D/teX Ultra		×		Normai	50	74
	XG_error_code	0 -			Theta/2-Theta				1	Fe	45	7
	🚼 X-ray	Off -		ak	🔚 XG power	Detector				_	-	
	🚼 Target	Cu(Ka) -			ZG_error_code				ð			
l	🕜 Tube voltage				X-ray	Detector # 1						
	Tube current				Target	HV:	0	V				
R	Shutter	Close -										
	Water flow	0.0 L/min -		Ĩ		PHA baseline:	38	div				
	Detector	Main Dete			Ube current	PHA window:	14	div				
	Data acquisiti				Shutter							
	DHA baseline	- 28 div -		<b></b>	🗃 Water flow	Dead time correc	tion					
	PHA window	14 div -			Detector							
	Count mode	Differential -			🗐 Data acquisiti	Tau int.:	0.7500	micro sec,				
(	Angle correcti	Disable -			HV # 1	Tau diff.:	0.2500	micro sec.				
	🔁 Angle correcti				PHA baseline	Corre	ct Not con	ect				
B	Slit correction	Disable -			PHA window							
Ē	Soller(inc.)	5.0deg -				Counter monochr	omator					
		10.0mm -			Count mode		Oth					
	₩ DS	1.250deg -			Angle correcti	€ Nd	U ND					
		8.0mm -			Angle correcti							
V	Soller(rec.)	5.udeg -			Slit correction	Register	Print	Close				
	Filter	K-beta(v2)			😴 Soller(inc.)							
	Monochroma	None -		<b>•</b>	IHS	10.0mm - I	=		1			
					Ξos	1.250deg -						
l					20	0.0mm						
۱				1	233		l					

18a Turning off the generator. Click Shutdown. In Shutdown window select XG Off. Click Execute



18b Turning off the generator. Once the generator is off the *Tube Voltage and Current* will be blank. In the *Shutdown* window click *OK*. Do not turn off the heat exchanger yet.



### 19a Exiting from MiniFlex Guidance.



19b Exiting from MiniFlex Guidance continued. After selecting *File*  $\rightarrow$  *Exit*, three message boxes will pop up.



20 Finishing up.

- 1. Remove your sample.
- 2. Turn off the diffractometer. Refer to the first slide.
- 3. Finish filling out the log sheet. Please enter total time as decimal hours.
- 4. Turn of the Haskris heat exchanger.
- 5. Log of the computer. **Do not Switch user**, **Sign out**!
- 6. And finally



Using the Google Calendar to Reserve the Diffractometer

Step 1. Add the Resource Calendar to your Google Calendar.

- Open your Google Calendar and scroll down the left side information until you come to "Other calendars". Click on the + symbol.
- Click on "Browse resources"
- Scroll down through the A-Z named resources until you come to "(Room)" and click on that.
- Check the box for ESS-GEO Room-245-25
- Return to your calendar
- You can make the ESS-GEO Room-245-25 calendar display on your calendar or not by giving it a distinct color and checking or unchecking the box next to it. When it is displayed, you should be able to see the details of existing reservations.

#### Step 2. Reserve the diffractometer

- Select a day/time in your Google Calendar giving it a title that includes 'XRD', your name and email address.
- Select the "Rooms" tab on the right hand side next to "Guests".
- In the search box below "Rooms", start to type "ESS-GEO" and you will see the resource calendar for ESS 245 show up in the results.
- Select the ESS-GEO Room-245 resource and save.

## Using Match! to Reformat Diffraction Data

7.1



**Step 1b.** Click on *Do nothing; wait for user actions ("Expert")* 



The Match! program is now loaded and ready.



A		
♦ Match!		
<u>File E</u> dit <u>V</u> iew <u>P</u> attern Pe	e <u>a</u> ks <u>S</u> earch E	intries Quantify Database Tools Options Help
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Open <u>r</u> ecent		
💾 Save	Ctrl+S	
💾 Save as	Ctrl+Shift+S	
<u>I</u> mport		Diffraction data
Export		Crystal struct Import powder diffraction data; insert as additional pattern(s) / overlays if diffraction data are already present
<u>C</u> ombine		Answer set
Print		Selection criteria
Print		Predefined phase selection Ctrl+Shift+O
🧹 Finish	Ctrl+W	Background
Run batch script		
File info		
% <u>Q</u> uit	Ctrl+Q	
500 -		

## **Step 2b.** Select your datafile. Choose the file with the extension *ras*.

l. 1000	Please select the diffraction data file(s) you would	d like to import/ir	isert:			×
950 -	← → × ↑ 📙 « Rigaku > miniflex > SiS	tandard		✓ <sup>5</sup> ✓	Search SiStandard	
900 -	Organize 🔻 New folder					. ?
850 -	Backup	^	Name     SiSettingJig-4-13-21.asc	Date modified 4/13/2021 11:42 AM	Type ASC File	Siz
800 -	baidwin		SiSettingJig-4-13-21.ras	4/13/2021 11:42 AM	RAS File	
750 -	convert		SiSettingJig-4-13-21.raw	4/13/2021 11:42 AM	RAW File	
	IntelFortran		SiStd-10Feb22.ras	2/10/2022 12:25 PM	RAS File	
700 -	KMS		SiStd-10Feb22_Theta_2-Theta.asc	2/10/2022 12:25 PM	ASC File	
650 -	LabVIEW Data		🔠 SiStd-10Feb22_Theta_2-Theta.raw	2/10/2022 12:25 PM	RAW File	
600 -	Match!		SiSettingJig-10Feb22.ras	2/10/2022 12:42 PM	RAS File	
	👌 Music		SiSettingJig-10Feb22_Theta_2-Theta.asc	2/10/2022 12:42 PM	ASC File	
550 -	Pictures		SiSettingJig-10Feb22_Theta_2-Theta.raw	2/10/2022 12:42 PM	RAW File	
500 -	Python3		SiSettingJig-3-31-22.ras	3/31/2022 10:26 AM	RAS File	
450	Recycle Bin		SiSettingJig-3-31-22_Theta_2-Theta.asc	3/31/2022 10:26 AM	ASC File	
450 -	Rigaku		SiSettingJig-3-31-22_Theta_2-Theta.raw	3/31/2022 10:26 AM	RAW File	
400 -	minifley		SiStandard-3-31-22.ras	3/31/2022 10:47 AM	RAS File	
350 -	registry		Sistandard 2.21.22 Theta 2 Theta raw	3/31/2022 10:47 AIVI	ASC FILE	
200		<b>.</b>	C Sistandard-3-31-22_meta_2-meta.iaw	5/51/2022 10:47 AIVI	NAW FILE	>
300 -						
250 -	File name: SiStandard-3-31-2	2.ras		✓ Any f	ile (*.*)	~

## Step 2c When the window Set Experimental Details appears, click OK



## Your diffraction pattern will be displayed.



## **Step 3a.** Select *File* $\rightarrow$ *Export* $\rightarrow$ *Profile data*

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Save as	Ctrl+Shift+S		
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Export	•	Pattern graphics	P3
<u>C</u> ombine	•	Profile data	
Print	•	Profile Export profile data of the current experimental pattern to a file	P5
Print	•	Profile data (Rietveld)	Pe
🖉 Finish	Ctrl+W	Background	P7
Run batch script		Peak data	
File info		Reflection data l(hkl) or  F(hkl)	
§ Quit	Ctrl+Q	Difference plot (profile)	Flor
		Pie chart (phase composition)	
500 -		Pie chart (elemental composition)	
450 -		Pie chart (phase and elemental composition)	
400 -		Entry data	
		Refined structure	
350 -		Reference pattern (peaks)	
300 -		Peak data (refined)	
250 -		Answer set (cand. list)	
200 -		Answer set (match list)	
		Selection criteria	
150 -		Peak list	
100 -		Candidate list	
50 -		Match list	
		Data sheet (original)	M. Pres
30.00	40.00 5	90.00 100.00 110.00 120.00 1	30.00 140.00
-Ka (1.541874 A)		Residual peaks	2theta

## **Step 3b.** For *Save as type* Select *Profile(2 columns: 2theta intensity) (\*.dat)* If need be, you can change the extension *dat* to something else.

🔶 Match!*			
<u>File E</u> dit <u>V</u> iew P	<u>P</u> attern Pe <u>a</u> ks <u>S</u> earch E <u>n</u> tries <u>Q</u> uantify <u>D</u> atabase <u>T</u> ools <u>O</u> ptions <u>H</u> elp		
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850 -	↑ Name Date modified Type	Size	P3 Na Mg
800 -	Desktop x No items match your search.		P4 K Ca Sc Ti V
750 -	Downloads		P6 Cs Ba La Hf Ta
700 -	Documents X		P7 Fr Ra Ac
650 -	GoogleDrive-KJB10		L Ce Pr
600 -	Google Drive (G:)		
500 -	MiniFlex		
450 -	Rigaku		
400 -	SiStandard		
350 -	OneDrive		
300 -	File name: SiStandard-3-31-22(dat)		
250 -	Profile (start, step, end, intensities) (*.dat) Profile (start, step, end, intensities) (*.dat) Profile (start, step, end, intensities) (*.dat)		
200 -	Hide Folders     Profile (2 columns: d-value intensity) (*.dat)     Profile (2 columns: 2theta intensity) (*.dat)		
150 -			
100 -			
50 -			Drosoti Neno / now sot

#### Step 3b Continued Click Save



Match! Continued: Preliminary data analysis



1.Click Peak List

## **2.** Click Options $\rightarrow$ General options

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## 3. Click Peak list

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V C	heck for availab	ble updates of the	e Match! software at	program sta	artup						
✓ C	heck for new or	· unused PDF dat	abases at program st	artup							
✓ A	utomatically sav	ve information fo	r restore	Interval [n	ninutes]:			0			
Defau	It selection pre	set: None / ne	ew set	*							
Exter	nal program pai	ths									
Diar	mond (structure	e visualization):	<undefined></undefined>			Modify	Download	Info			
End	leavour (structu	ure solution):	<undefined></undefined>			Modify	Download	Info			
Full	Prof (Rietveld r	efinement):	<undefined></undefined>			Modify	Download	Info			
Tre	or (indexing; ind	d. in FullProf):	<undefined></undefined>			Modify	Download	Info			
Dicv	/ol (indexing; in	d. in FullProf):	<undefined></undefined>			Modify	Download	Info			

## **4.** Select *2Theta/d-values* then click *OK*

Match! O	ptions											2
General	Raw data	Search-Match	Quant. analysis	Batch	Graphics	Peak list	Candidate list	Match list	Rietveld	Data sheet	Indexing	
Display (	peak data of co	orrelated reference	peaks as:	۲	2theta/d-valu	ies (	Intensities					
21	theta O	d 🔿 1/d										
	4.6.1				· · · ·							

5. Click Icon for *Strip K-Alpha2*. Notice changes in the diffraction pattern. Like here.



## 6. Click Subtract background and look for changes in pattern again



7. Click on Icon for *Run phase identification (search-match)* 



#### 8. Observe Peak list

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Eile Edit	Viev	w <u>P</u> attern P	Pe <u>a</u> ks <u>S</u> earch ⊗a ⊨ I. <mark>vl</mark>	Entries Qua	antify <u>D</u> atabas	ise <u>T</u> ools <u>O</u>	ptions <u>H</u> elp		<b>-</b> 1 <b>- - - - - - -</b>		an - I 🙃 ka	- 0								
ii 🛄 🚄							* • • •	we rr 🜒 📑	• • • (*	· 🕒 🧧	~~ : : 🖤 🖻	1 0 <del>4</del>		2theta	Peak height	EWHM	96-901-1	999		
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1000 -											SiStandard-3-	31-22		47.34	718.8	0.1074	47.30	)		
950 -											Calc. (exp. pe	aks) (Rp=22.9	9%)	56.16	414.3	0.1012	56.12	2		
1											Background			56.42	6.7	0.0600				
900 -	•••••										[96-901-1999]	SI Silicon		69.16	95.9	0.1098	69.13	3		
850 -														76.42	163.9	0.1091	76.38	3		
														88.06	207.3	0.1151	88.03	}		
800 -														88.56	2.7	0.3259				
750														94.98	108.2	0.1210	94.9	5		
/50-														106.74	67.6	0.1286	106.7	1		
700 -														114.12	119.9	0.1378	114.0	9		
														127.58	104.1	0.1633	127.5	5		
650 -														136.92	57.4	0.1847	136.8	9		
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	C	96-901-1999	Si			С	Silicon		0.9959	0.9753	0.9338	4.39	0.9904							
	C	96-410-4918	Si			С			0.9951	0.9678	0.9188	4.45	0.9892							
	C	96-900-8566	Si			С	Silicon		0.9897	0.9753	0.9338	4.39	0.9889							
	C	96-900-8567	Si			С	Silicon		0.9897	0.9753	0.9338	4.39	0.9889	Do	uble-click or o	lrag entries h	here to select	them as 'matching'	•	
	C	96-210-4738	Si			С	Silicon		0.9962	0.9466	0.8883	4.57	0.9868							
	C	96-210-4749	Si			С	Silicon		0.9962	0.9465	0.8882	4.58	0.9868							
	C	96-901-3103	Si			С	Silicon		0.9770	0.9753	0.9338	4.39	0.9859							
	C	96-101-1234	Fe0.34 S Zn0.66	5		С	Zinc iron sulfide (.7	/.3/1) (Sphalerite (F)	0.9963	0.9397	0.9619	8.74	0.9546							
	C 96-154-1432 Ca Cd F8 Na Y		С	Na Ca Cd Y F8		0.9769	0.8901	0.8515	6.42	0.9434										
1	C 96-210-2764 Si				С			0.7238	0.9635	0.9109	4.49	0.9241								
4	C 96-153-8544 Cd0.9 F2.1 Tb0.1				C Cd0.90 Tb0.10 F2.10															
	C	96-153-8544 Cd0.9 F2.1 (b0.1 96-154-1646 Ce0.66 O2 U0.34				С	Cd0.90 Tb0.10 F2.	10	0.9082	0.7356	0.9397	12.48	0.9092							

## Manually mapping to your 'mysbfiles'

1. Open File Explorer and right click on *This PC* and select *Map network drive…* 



2. Select a *Drive letter* and the *Folder*: <u>\\mysbfiles.campus.stonybrook.edu\*NetID*</u> Be sure to replace NetID with your actual NetID. Click *Finish*