How to start an experiment at BT7

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- 1. To start JICE, find the "JICE-month-date-year.jar" icon (for example, ^{7372008,jar}) on the BT7 desktop. Double-click the icon to start the client. All commands to the instrument are executed from the JICE program.
- 2. The BT-7 *Instrument Scientist* (as a 'superuser') can set up a subdirectory for the experiment. In the JICE window, under "File", choose "new experiment" and a pop up window will open. (S)he will enter the proposal ID of the new experiment. Then the "experiment configuration" window pops up with the "Experimental details" tab open (there are three tabs). Under the "Experimental details" tab, you can enter "experiment name", "participants" and "experiment details". Under the "sample environment" tab, you can set up the temperature and/or magnetic field controllers for your particular sample environment. Click on "controller type", pick "Temp" or "Magfield", for example, then click on "controller" to see a list of controllers, then Press "Add Device". You can also "update device" if some 'under-the-hood' device parameters need to be changed, or "remove device". You also can change software limits under the "device details" tab, but this must be done with great caution; these limits are there to protect the instrument, so please do not increase the limits unless you are absolutely certain that no problems can occur. In general, you should NOT increase the limits.

Users can access the experimental configuration information under "Edit", then "Experiment configuration".

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/ Server Queue) Samp		
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Alghment Mode.		1
Setting Up the O		
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Approximate latti		
For reference: α i	9	
a: 6.2832 Å		
α: 90.0 *		
		Apply Reset
	Setup for adding, removing, and updating a controller for the sample environment.	
Scattering Plane	Devices on System	
Enter two non-col		
plane.		
h1: 1.0 k	·	Apply
	Controller Type Controller Alias	
h2: 0.0 k	Temp 🔹 lakeshore331 🔹 Temp	Reset
	Properties	
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A3		- 0.1 +
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To define the scatt		
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Elastic scattering a		
h:		
		nent Position Θ(A3):N/A
		5(AS).11/A
a) Run a O (A3) pe	Red indicates a required field OK Cancel	
c) run an Upper T		
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3. Many of the instrument operations can be accessed through the various windows. Requesting a

		Premonocal OPEN Filter Focus DUT Mono Focus (HV) PLAT/SGTL Analyzer Mode FLAT Detector Mode <u>5D</u> ICP Data on
		Internal we
E Conso	le - JICE	
File Edit	Window Help	
	Console	Instrument State: PAUSE 😡 😏
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	Peak Scan	Instrument Time: Tue Sep 16 10:50:34 EDT 2008
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Curre	Resource Manager	A)
	Sample Alignment	Scan Progress: No scan running.
	Server Queue	
Log Mess	ages Dry Run Results	Detailed Error Messages
10:50:2	1 AM> ask GETFITE	ESULTS getnewlattice
		-

window, such as "Live Data", will create a new tab with that window active in the Console. These tabs can also be dragged out onto the desktop as a stand-alone window, if desired.

The icon at the top of the desktop gives some basic instrument information, and can be used to *pause and resume*, or *stop* the instrument command sequence. This icon appears on all the desktops and is forced to the front so that it is always available. The keyboard command "ALT-F12" can also be used to stop the instrument.

4. To input lattice parameters and align your sample, choose the "sample alignment" tab.

	Mon Sep 15, 17:37	Premonocoli OPEN Filter Focus OUT	Instrument: BT7	3 🥹 🥸 84 °F 🔂 🔳	🔲 🚱 🔁 🏩 😒 🐟 🕴 İndiv
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	Sample Align	nent - J Detector Mode SD			
ile Edit Window H	leip				
Server Queue \ Sample >	Alignment \ 🚍 Console \ 🛟 Move Device '		ient State: PAUSE 😣 😔 itor \		
Nignment Mode: UB Ma					
Cotting Up the Orier	ntation Matrix for the Sample				
	ants and angles that describe the structure	e of the crystal lattice for your sample.			
Approximate lattice s	pacings can be entered and later refined e angle between a and b, β is the angle b	after scanning 20.	een cand a		
a: 6.2832 Å b:	6.2832 Å C 6.2832 Å				
α: 90.0 * β:	90.0 • Y: 90.0 •				
			Apply Reset		
Scattering Plane Def					
Enter two non-colines plane.	ar reciprocal lattice vectors to define the s	cattering			
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h2: 0.0 k2:	0.0 12: 1.0		Reset		
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Move Devices					
Device	CurrentPosition Targ	etPosition	Jog Step		
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A3	35.915° 35.9	146 Go!	- 0.1 +		
Align Sample at Latti	ice Reflection(s)				
To define the scattering	ng plane, a minimum of two reflections mu				
Repeat this for any nu	lection desired and fine tune the location i mber of reflections until you are confident				
plane is defined.					
Elastic scattering assu					
h: k:		Drive A4 Drive Q (A3/A	44)		
		Calculated Angular Alignm 20(A4):N/A	ent Position 0(A3):N/A		
a) Run a O (A3) peak		n a 0/20(A3/A4) peak scan			
c) run an Upper Tilt o	or Lower Tilt peak scan				
🚱 Server Queue -	- JICE				

- a) Enter "a", "b", "c", " α ", " β " and " γ " and click on "apply" to define crystal lattice.
- b) Enter "*h1*", "*k1*", "*l1*" and "*h2*", "*k2*", and "*l2*" and click on "**apply**" to define the scattering plane.
- c) Enter "*h*", "*k*" and "*l*", and JICE will calculate and display the A4 (diffraction angle), and A3 (sample rotation) values. If this is your first peak, press "drive A4" to move the analyzer system to the correct Bragg angle. Then go to the "move device" window to drive "A3"

around until you find your peak.

- d) To do a rocking scan, open the "peak scan" window. Then choose device "A3", and enter values for "range", "step size", "duration" and click on "findpeak". You can "move to fit" and then "redefine A3" to the calculated value shown in the "sample alignment" panel. You determine the actual d-spacing by doing an "A3-A4" (θ:2θ) and then update the appropriate lattice parameter(s), and adjust the goniometer tilts by scanning "smplutilt" or "smpltilt" [sample upper tilt, sample lower tilt] in the peak scan panel.
- e) Once your first peak is properly aligned, input the (*h*,*k*,*l*) for the second peak and go to the 2nd peak via the "sample alignment" panel (enter "*h*", "*k*", "*l*" and press "drive to Q"). Adjust the tilt (peak scan on "smplutilt" or "smplltilt") and adjust the lattice parameter(s) for this peak ("peak scan" on "A3-A4").
- 5. Once sample is aligned, you can adjust the width and height of slits before the sample ("smplwdth" or "smplhght") and after the sample ("bksltwdth" or "bkslthght") ("peak scan" these four motors one by one), to reduce your background.
- 6. To set up a scan, go to "File", and "New". Choose either "Angle scan", "motor scan", "vector scan" or "environmental scan".

Console - JICE		
File Edit Window Help		
New	Angle Scan	Instrument State: PAUSE 😣 🥑
Open	Vector Scan	
Close	Environment Scan	
Save	Motor Scan	Instrument Time: Tue Sep 16 10:52:37 EDT 2008
Save As	Sequence	
Print	run by N/A)	
Reconnect	Scan Progress	No scan running.
Change Instrument		
Change Experiment		
Administrative Mode	s Detailed Error Messages	
Exit	TRESULTS getnewlattice	

A new tab will open to allow you to set up that type of scan. You can choose either to enter "initial/final", "initial/step" or "center/step" values.

a) To do a "motor scan", click on the little square before the motor of interest, enter "scan ranges", "number of points", and "base count" (to measure the monitor rate go to "console panel" and type "rate" at the command line) and "prefactor", then give your scan a "scan name"; The scan name will be used to actually execute the scan. The data file will be saved using the "data file prefix" as the filename prefix plus a number. Enter "comments" if desired. Press "save scan" to save it, "dryrun scan" to calculate the angles and check angle limits, and "save and run scan" to run the scan manually. Dryrun will open a pop-up window to view the angles and error messages (if any), and the results of the Dryrun will also appear in the Console Tab. Running the scan puts the command in the server queue (explained below) to be executed.

Sample Alignment	🛓 Live Data 🙀 *Untit	led1			Instrument	State
strument						
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	Initial	Final	Center	Step	Units	
Ai 🗌][N/A	N/A		
🗖 A2		10	N/A	N/A		
EA 🗌			NIA	N/A		
A4	10	20	15	0.2		
A5		1	NIA	N/A		
A6		1	N/A	N/A		
Additional Devices						
Include Amother D	Vevice in Scan					
Scan Parameters						
	Number of Points:	51	Data of Interest:	Detector 💌		
	Base Count:	1	Count Against:	Time 💌		
	Prefactor:	1	Timeout:			
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- b) To do a scan of a Bragg peak (a.k.a. Bragg Buffer in ICP), in "motor scan" choose "center/step" mode, go to the section called "Bragg Buffer", enter "Et=ei-ef" 0 meV and enter the value for "fixed Ei/Ef". Enter "*h*,*k*,*l*" then press "populate fields" and all the values for the angles are populated. To do an A3 (rocking) scan, click on the square before A3; To do an A3:A4 (θ:2θ) scan, click on the square before A3 and A4, and enter the steps for A3 and A4 in a 1:2 ratio.
- c) To do a constant-Q or contant-E scan, go to "vector scan" and enter values for "*h*", "*k*", "*l*" and "E", enter "scan name", "data file prefix" and "comments". Press "save

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rver Queue 58	ple Alignment \ 🚍 Console \ 🏠 Move Device \ 🔟 Live Data \ Peak Scan \ Resource Editor \ i or other position in reciprocal space) along a vector direction.	onuted
	Instrument	
	Fixed Energy Fixed Ef 🔹 14.7 meV	
	Mode: Mode: Initial/Final Initial/Step Center/Step	
	Initial Final Center Step Units	
	h 2.0 2.0 2 0 rlu	
	k 0.0 0.0 0 rlu	
	I 0.0 0.0 0 0 riu	
	Scan Parameters Number of Points: 31 Data of Interest: Detector	
	Base Count: 170000.0 Count Against: Monitor -	
	Prefactor: 1.0 Timeout:	
	Environment Environment parameter will be set to target value before scan is started.	
	Any device with fields left blank will not be moved and will stay at whatever	
	the current position is at run time.	
	Controller Type: Please Select Device	
	Properties	
	Scan Description	
	Scan Name: Q2	
	Data File Prefix: YHoMnO3	
	Comments:	
	✓	
	Clear Dry Run Scan Save Scan Save and Run Scan	

scan" to save it, "dryrun scan" to "dry run" or press "save and run scan" to run the scan.

- d) To do an environment scan such as scanning the temperature or magnetic field, choose "environment scan". Select either "Temp" or "Hmag". Enter the appropriate ranges, and go to "properties" to enter the values for "tolerance", "wait between the points", "wait before the points". NOTE: Make sure to move to the correct A4 value or Bragg position of interest before running the environment scan.
- 7. To run a sequence of scans, go to "window", then "server queue". On the left of the server queue window, there is folder called "scans" and your scans are saved there. To execute a scan you can either 1) click on the scan of interest, then drag to the right window, OR 2) right click on the scan and the choose "add to queue". "scan runscan <scanname>" will show up in the server queue in the right pane of the window. If this is the first scan in the queue, then this scan will start running and "scan runscan <scanname>" becomes bold. Drag additional scans into the queue in the order you want. Any other commands that you want to execute, such as "move temp 231.0", can be executed from the console command line, or any of the other command windows such as in "move device" or "find peak", and these will be added to the queue in the order in which they are given. You can change the order in the move them up or down by pressing the "up" or "down" buttons, or remove them with the "remove" button.
- 8. Alternatively, you can write a sequence file. Go to "file", then "new", then "sequence", then a sequence tab will open. You can write all the commands in this file, then go to "File", then "save" or "save as" to the filename of your choice. Then go to the "server queue", and in the

left pane there is a "sequence" folder and your sequence file is saved there. Drag the sequence file to the right pane, or right click and choose "add to queue" to run the sequence file. Current data are displayed in the "live data" panel.

Server Queue \ Sample Alig	nment 🔪 🚍 Console 🕽 🛟 Move Device 🕽 💹 Li	Instrument State: PAUSE
iles		The Data (Teak Scall (Resource Editor)
→ Files →	Current Point: N/A Total Points: 1	Monitor Count: N/A Detector Count: N/A
Q2.5 Q4 Q4 Q4 Q4 Q4 Q4 Q4 Ben.seq.txt Ben.seq.txt Sill.seq.txt Python Scripts Common	Z:scan runscan Q2 3:scan runscan Q2.5 4:scan runscan Q3	Re
stimated time to completion		

9. To get your experimental data onto your own computer, you can use a memory stick at BT7 to copy your data. The data directory is located at /usr/local/ice/usr/<proposalID>/data . Alternatively, if you are on the visitor's network in the user room, you can find your data on the charlotte computer. You can get to charlotte by typing <u>\charlotte.ncnr.nist.gov</u> in the address bar of any window. All data are archived here and are organized in subdirectories by the year and month that the cycle started. auto-mounted on your computer (if not, open network places, and go to charlotte.ncnr.nist.gov). Go to the "ICP data" subdirectory, go to "BT7". Then go to the latest folder (e.g. 200807, for the cycle that started July, 2008), then to the folder with your proposal ID number. You can copy (select and drag/copy) your data to your own computer. DAVE can be downloaded at <u>http://www.ncnr.nist.gov/dave/download.html</u> onto your laptop to view and analyze your data, or you can use your own software. All triple axis data are stored as simple ascii files.