

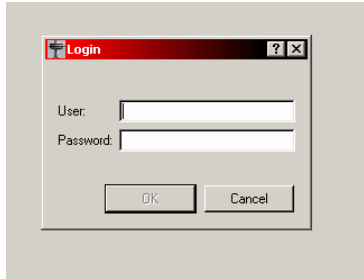
# Data Collection on the APEXII

Instructor : Joseph H. Reibenspies

Version 1.0.0

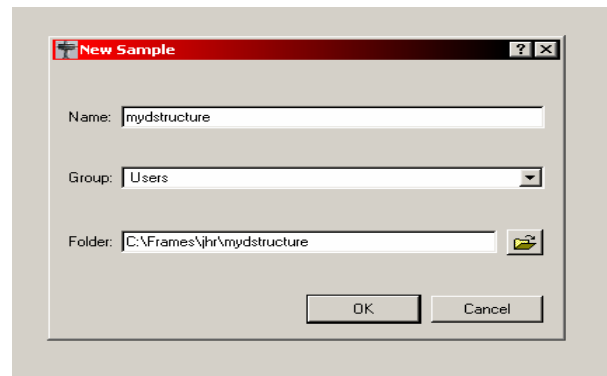
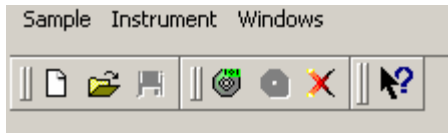
# Data Collection on the APEXII

## 1. Login

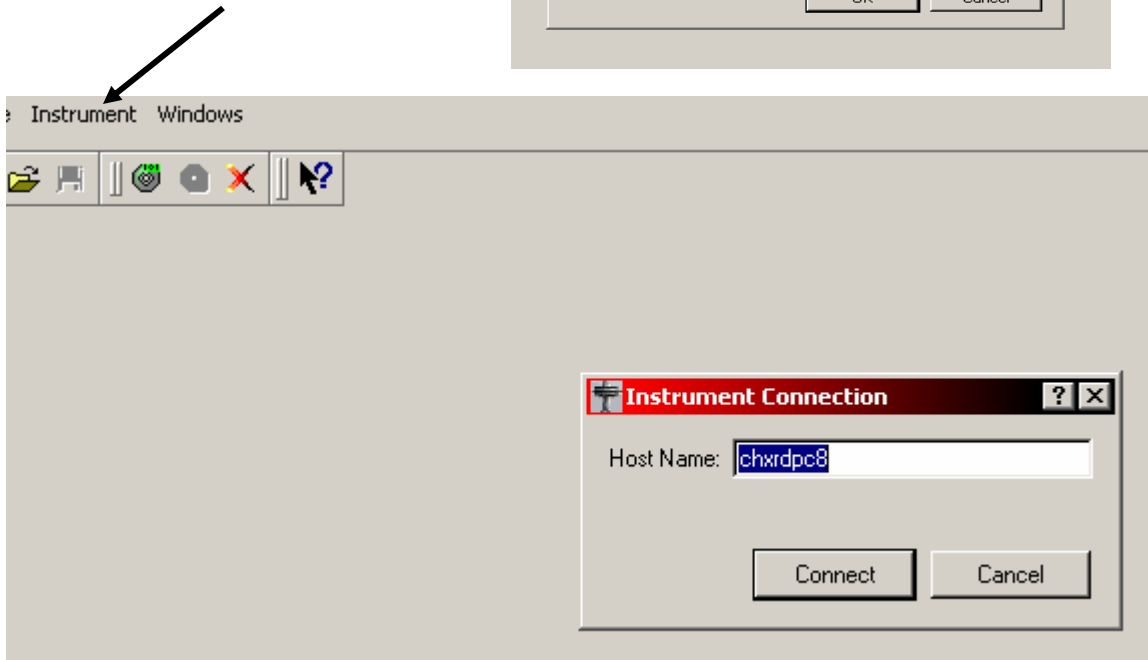


User name and password will be supplied to you

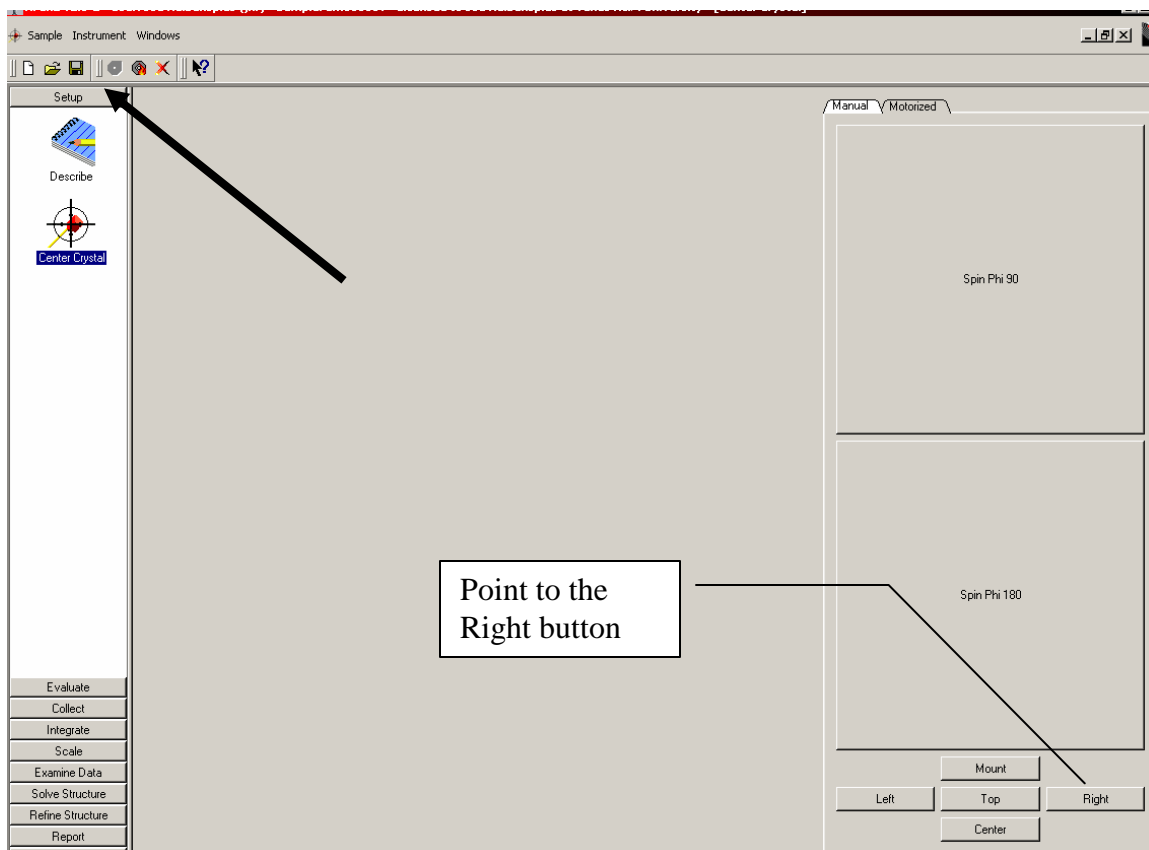
## 2. Start a new project



## 3. Connect the computer



#### 4. Center Crystal



## 5. Determine Unit Cell

APEX2 v2.0-2 - User: Joe Reibenspies (jhr) - Sample: test2 - Licensed to Joe Reibenspies at Texas A&M University - [Determine Unit Cell]

Sample Instrument Windows

Setup

Evaluate

Determine Unit Cell

Transform unit cell

Reciprocal Lattice Viewer

View Images

Collect

Integrate

Scale

Examine Data

Solve Structure

Refine Structure

Report

Instrument

Cursor

- Position [mm]
- Position [pixels]
- Intensity [counts]
- HKL index
- Resolution [Å]
- 2Theta [°]

Image Header / Tool Editor / Cursor Position

Automatic Mode

Start at: Collect Data

Stop after: Refine

Run

Manual Mode

Collect Data

Harvest Spots

Index

Brevis

Refine

Unit cells:

Edit...

Delete

Delete All

Reflections:

Edit...

Delete

Delete All

Expected resolution:

	Exposure time [s]	Resolution [Å]
1	20.0	n/a
2	60.0	n/a
3	120.0	n/a
4	600.0	n/a

Crystal Mosaicity [°]: 0.40

## 6. Start Data Collection

The screenshot shows the 'Monitor Experiment' window. A table lists operations from 1 to 27. A 'Load Experiment' dialog box is open, showing a file explorer view of 'C:\Frames\' with 'short\_run.exp' selected. Callouts indicate the following steps:

- Point to Collect:** Points to the 'Collect' button in the left sidebar.
- Point to Experiment:** Points to the 'Experiment' button in the left sidebar.
- Find short\_runs:** Points to the 'short\_run.exp' file in the 'Load Experiment' dialog.
- Point to Load Table:** Points to the 'Load Table...' button at the bottom of the main window.

Operation	Active	3	4	5	6	7	8	9	10	11
1	No Operation	Yes								
2	No Operation	Yes								
3	No Operation	Yes								
4	No Operation	Yes								
5	No Operation	Yes								
6	No Operation	Yes								
7	No Operation	Yes								
8	No Operation	Yes								
9	No Operation	Yes								
10	No Operation	Yes								
11	No Operation	Yes								
12	No Operation	Yes								
13	No Operation	Yes								
14	No Operation	Yes								
15	No Operation	Yes								
16	No Operation	Yes								
17	No Operation	Yes								
18	No Operation	Yes								
19	No Operation	Yes								
20	No Operation	Yes								
21	No Operation	Yes								
22	No Operation	Yes								
23	No Operation	Yes								
24	No Operation	Yes								
25	No Operation	Yes								
26	No Operation	Yes								
27	No Operation	Yes								

## 7.

The screenshot shows the 'Monitor Experiment' window. A table lists operations from 1 to 27. A 'Load Experiment' dialog box is open, showing a file explorer view of 'C:\Frames\' with 'short\_run.exp' selected. Callouts indicate the following steps:

- Data file name:** Points to the 'Filename or prefix' field containing 'data'.
- Change Data collection time:** Points to the 'Default time' field containing '10.000'.
- Start Data Collection:** Points to the 'Execute' button at the bottom right.

Operation	Active	Distance [mm]	2Theta [deg]	Omega [deg]	Phi [deg]	Chi [deg]	Time [sec]	Width [deg]	Sweep [deg]	Direction
1	Generator	Yes	50.000				40.000			
2	Omega Scan	Yes	60.000	-28.000	-28.000	0.000	54.736 default	default		180.000 negative
3	Omega Scan	Yes	60.000	-28.000	-28.000	90.000	54.736 default	default		180.000 negative
4	Omega Scan	Yes	60.000	-28.000	-28.000	180.000	54.736 default	default		180.000 negative
5	Omega Scan	Yes	60.000	-28.000	-28.000	270.000	54.736 default	default		180.000 negative
6	No Operation	Yes								
7	No Operation	Yes								
8	No Operation	Yes								
9	No Operation	Yes								
10	No Operation	Yes								
11	No Operation	Yes								
12	No Operation	Yes								
13	No Operation	Yes								
14	No Operation	Yes								
15	No Operation	Yes								
16	No Operation	Yes								
17	No Operation	Yes								
18	No Operation	Yes								
19	No Operation	Yes								
20	No Operation	Yes								
21	No Operation	Yes								
22	No Operation	Yes								
23	No Operation	Yes								
24	No Operation	Yes								
25	No Operation	Yes								
26	No Operation	Yes								
27	No Operation	Yes								

## 8. Crystal Face

Unit Cell

$a=31.93\text{\AA}$ ,  $b=16.31\text{\AA}$ ,  $c=16.35\text{\AA}$   
 $\alpha=90.00^\circ$ ,  $\beta=94.27^\circ$ ,  $\gamma=90.00^\circ$   
 $V=8493\text{\AA}^3$ , Monoclinic C

H	K	L	Distance [mm]
0	1	0	0.21
0	-1	0	0.26
0	0	1	0.03
0	0	-1	0.02
1	0	0	0.05
-1	0	0	0.07

Remove Invisible Faces

Closed:  Yes

Size [mm]: 0.06 x 0.14 x 0.52

Crystal Face  
 Miller Indices: 0 0 1  
 Distance [mm]: 0.26  
 Out-of-plane angle [deg]: 0.74

Max. Miller index: 2  
 Max. out-of-plane angle [deg]: 1

Show T-tool  
 Show possible face normals  
 Snap to possible face normals

Unit Cell

$a=31.93\text{\AA}$ ,  $b=16.31\text{\AA}$ ,  $c=16.35\text{\AA}$   
 $\alpha=90.00^\circ$ ,  $\beta=94.27^\circ$ ,  $\gamma=90.00^\circ$   
 $V=8493\text{\AA}^3$ , Monoclinic C

H	K	L	Distance [mm]
0	1	0	0.21
0	-1	0	0.26
0	0	1	0.03
0	0	-1	0.02
1	0	0	0.05
-1	0	0	0.07

Remove Invisible Faces

Closed:  Yes

Size [mm]: 0.06 x 0.14 x 0.52

Crystal Face  
 Miller Indices: n/a n/a n/a  
 Distance [mm]: n/a  
 Out-of-plane angle [deg]: n/a

Max. Miller index: 2  
 Max. out-of-plane angle [deg]: 1

Show T-tool  
 Show possible face normals  
 Snap to possible face normals