ORIENTEXPRESS

Test Laue neutron-diffractometer

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Return to Viewing and indexing data

CLIP (COLOGNE LAUE INDEXATION PROGRAM)

CLIP ("Cologne Laue Indexation Program") is written by Olaf Schumann.

It may be freely downloaded at https://clip4.sourceforge.net.

CLIP is installed on the Windows 10 machine. It may be started by double-clicking in the CLIP icon.

Help menu:

CLIP tutorial

Useful tools:

- Reorientation: How far are you from perfect alignment?
- Rotation: What happens if I rotate the crystal?
- Reflection Info: Interrogate the indexed peaks

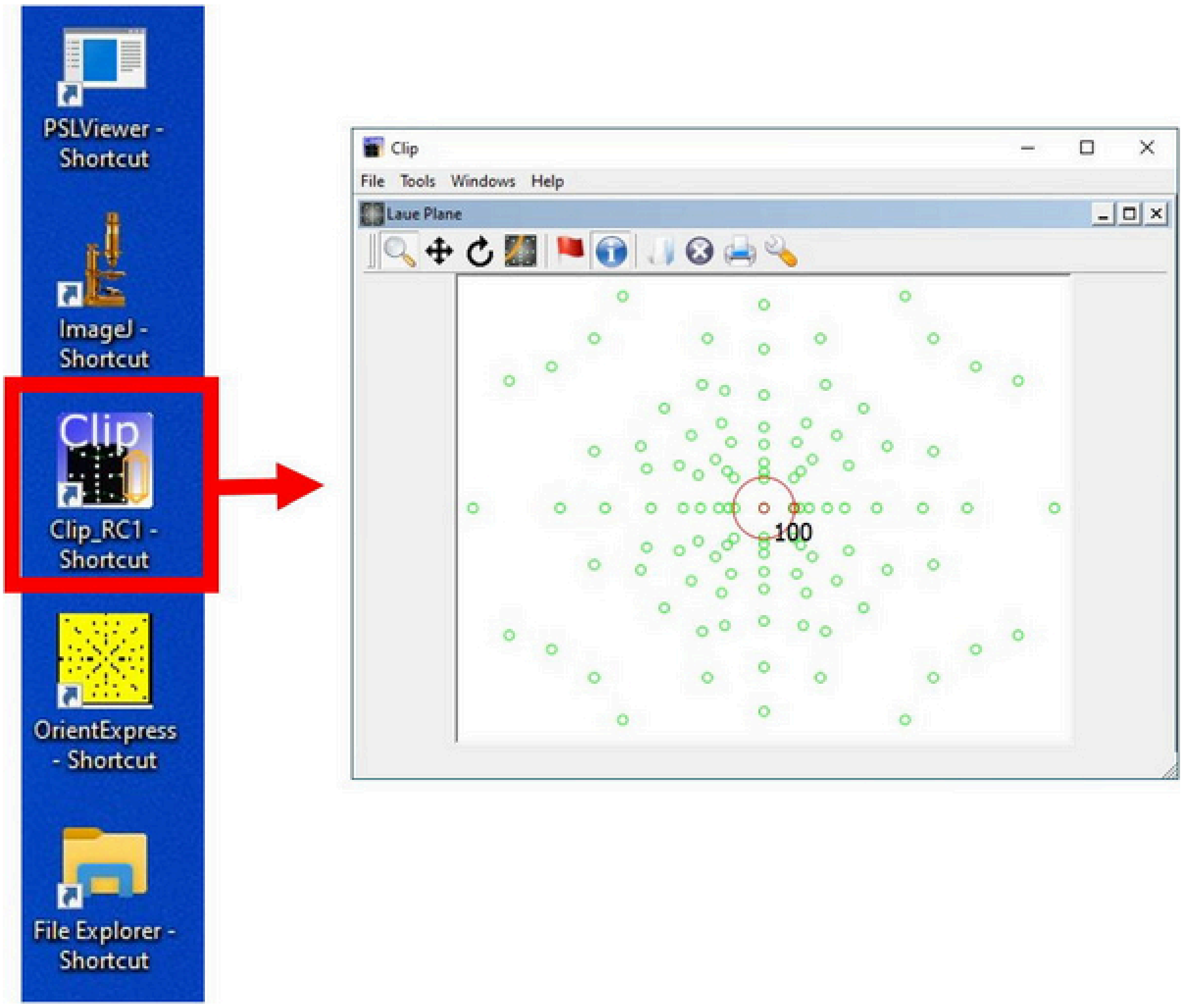
Click here (pdf - 0.91 Mi) for the CLIP manual.

CLIP tutorial

CLIP requires the data to be in **PNG** or **BMP** format. Use ImageJ to convert the TIF data to these formats,

1. Start CLIP

Start CLIP by clicking on the appropriate icon on the Windows 10 computer.

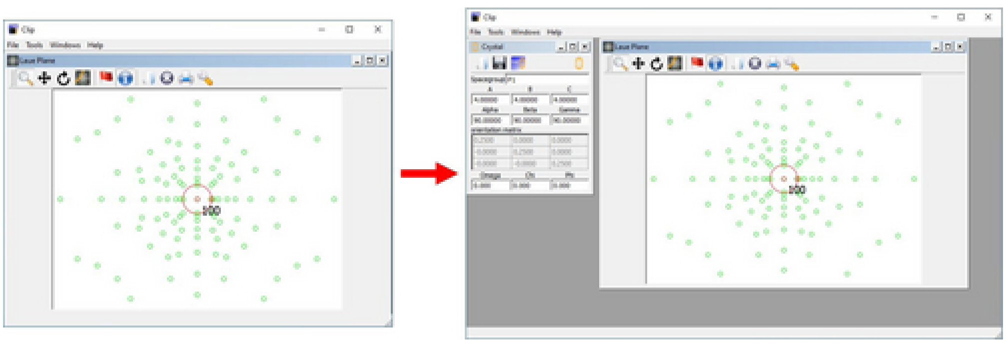


2. Set the windows

The **CLIP** window contains sub-windows. The **Laue Plane** window is in the foreground, and there is a **Crystal** window hidden behind it.

Stretch the **CLIP** window by clicking and draging the bottom left corner.

Move the **Laue Plane** window to one side to reveal the **Crystal** window.

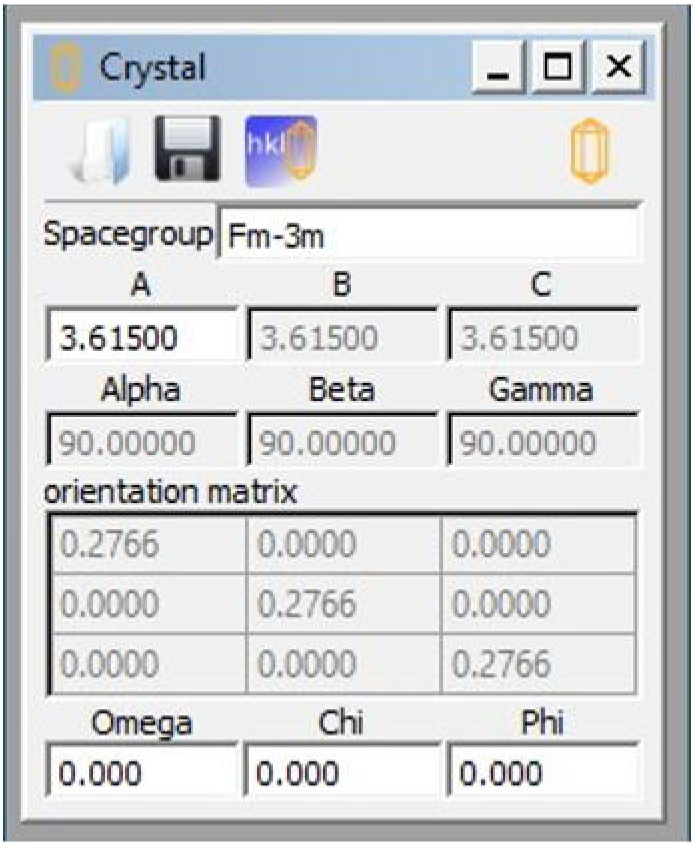


3. Set the unit cell

Select the **Crystal** sub-window.

Enter the correct space group and lattice parameters.

The orientation matrix and values for *Omega* , *Chi* and *Phi* are unimportant for the moment.



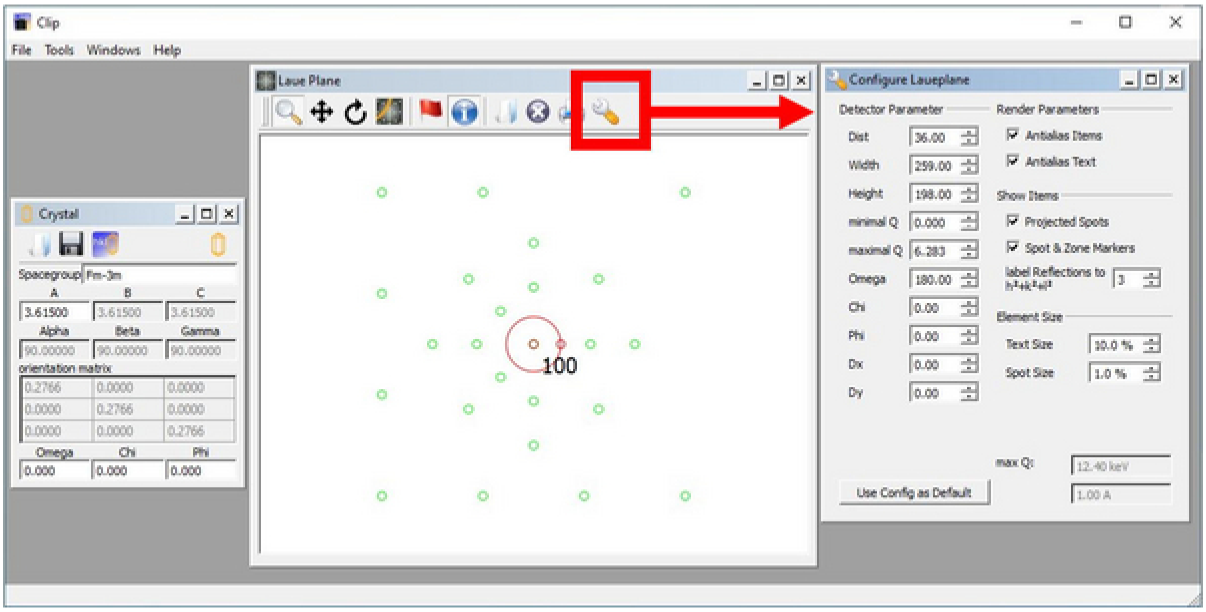
If the unit cell window is closed, a new one may be opened from the **File : New Crystal** menu option.

4. Set the instrument configuration

Access the **Configure Laueplane** window by clicking the 'spanner' icon in the **Laue Plane** window.

The detector **Width** = 259 and Height = 198.

Pay particular attention to **Dist**, which is the sample-detector distance. The correct value is given by the '*Horizontal*' motor axis in NOMAD.

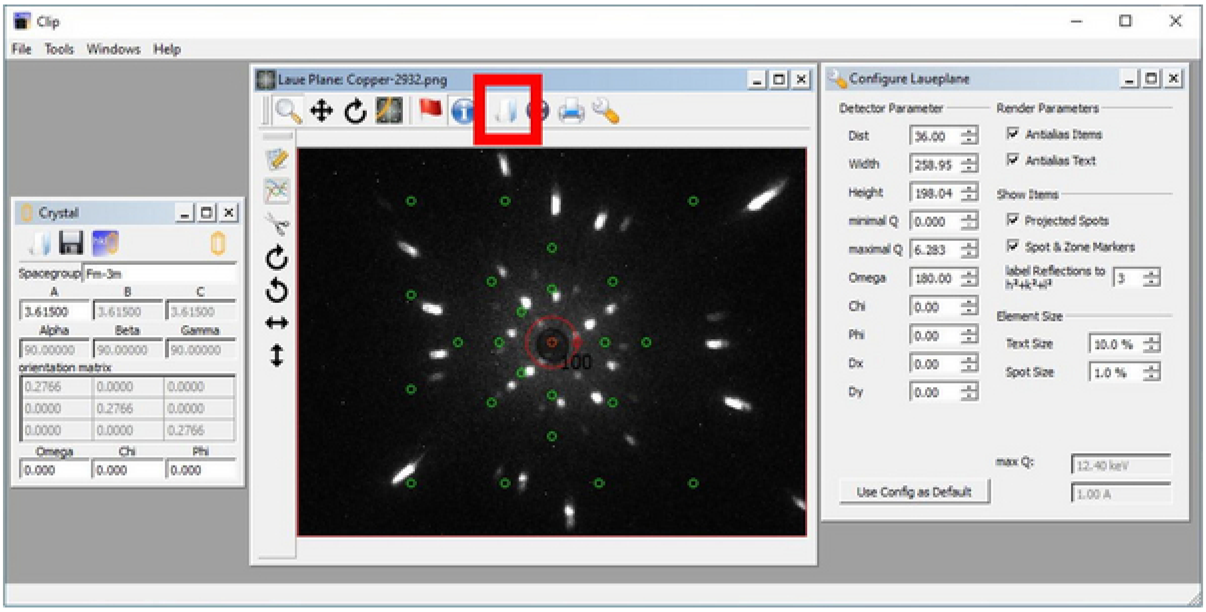


If the **Laue Plane** window is closed, a new one may be opened from the **File : New Laue Plane** menu option.

5. Load the data

This is done by clicking the 'Book' icon in the **Laue Plane** window.

Be sure that you are loading a PNG or BMP file.



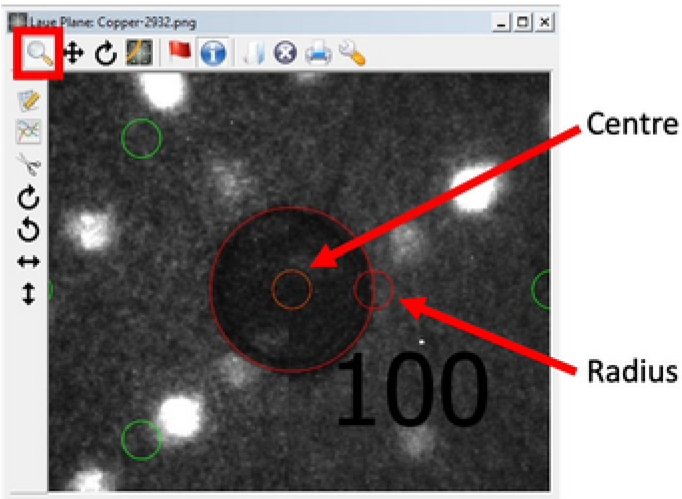
6. Define the main beam position

The main beam is defined in the **Laue Plane** image with a red circle.

The circle may be *moved* by clicking and dragging the smaller circle in its centre.

The circle *radius* may be changed by clicking and dragging the smaller circle on its circumference.

The image may be *zoomed* by using the *magnifying glass* icon in the **Laue Plane** window. Right-click in the image to reset the zoom.



7. Define some Laue zones

Use the *Zone* tool in the **Laue Plane** window to define some Laue zones.

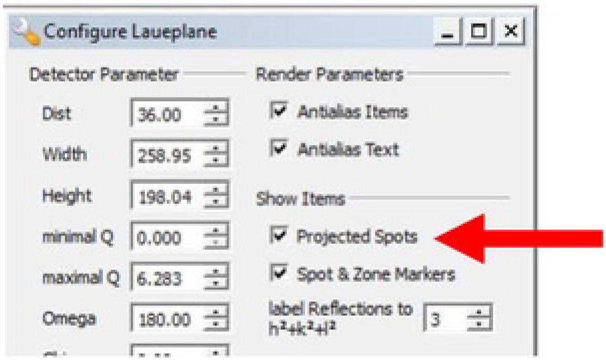
With the tool active, click on a peak position and drag to another peak on the same trajectory.

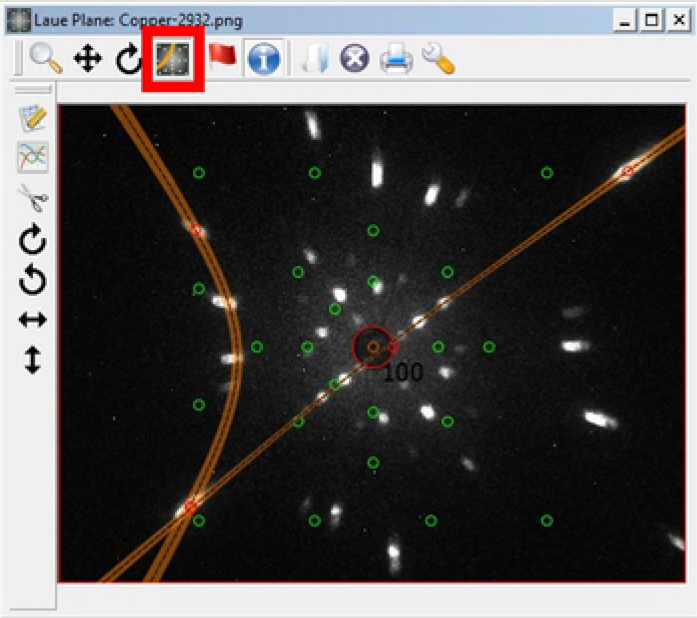
A line will appear on the image.

The line contains two small red circles. The line can be modified by clicking and dragging one of the circles, or deleted by right-clicking on a circle.

Select at least three zones before attempting to index.

The *green circles* show the projected spots. You can toggle their visibility from the **Configure Laueplane** window.





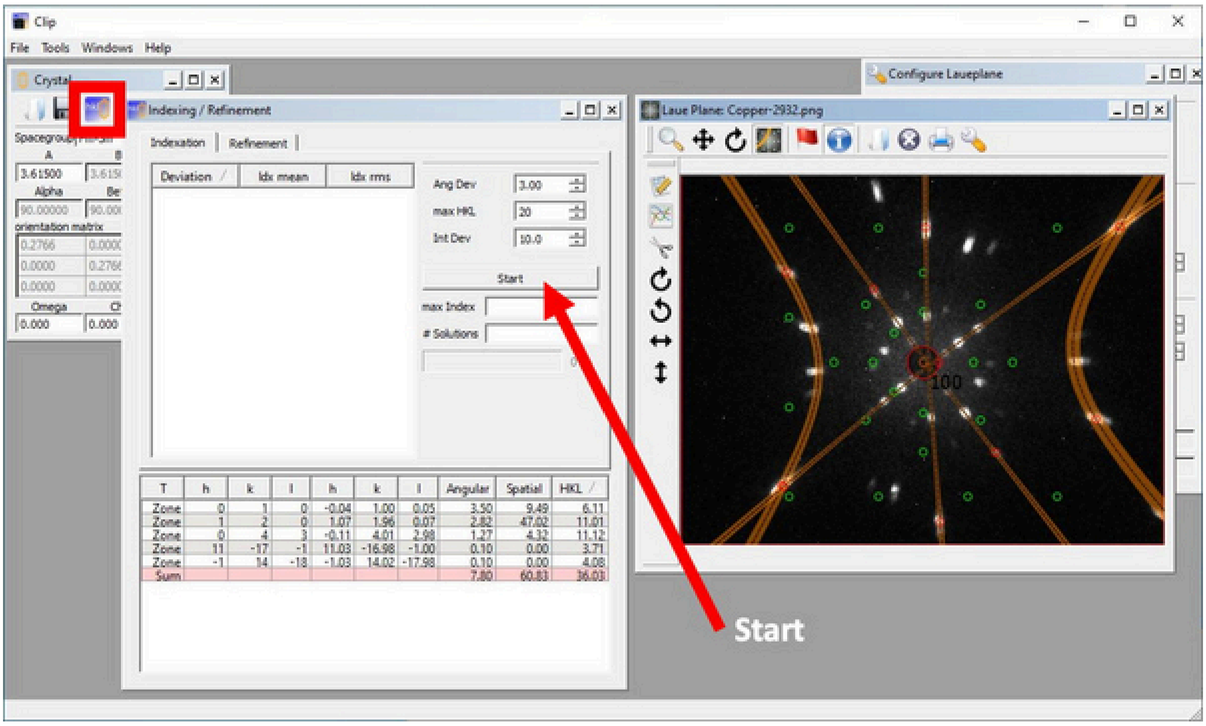
8. Start indexing

Open the **Indexing / Refinement** tool by clicking on the *hkl* icon in the **Crystal** window.

The windowhas a *Start* button. Click this button to *start and stop* the indexing.

CLIP will not stop indexing on its own. If it runs for too long, CLIP will run out of memory and will crash.

YOU must be the one to stop the indexing. Letting CLIP run the indexing for ~1 - 3 seconds is about right.



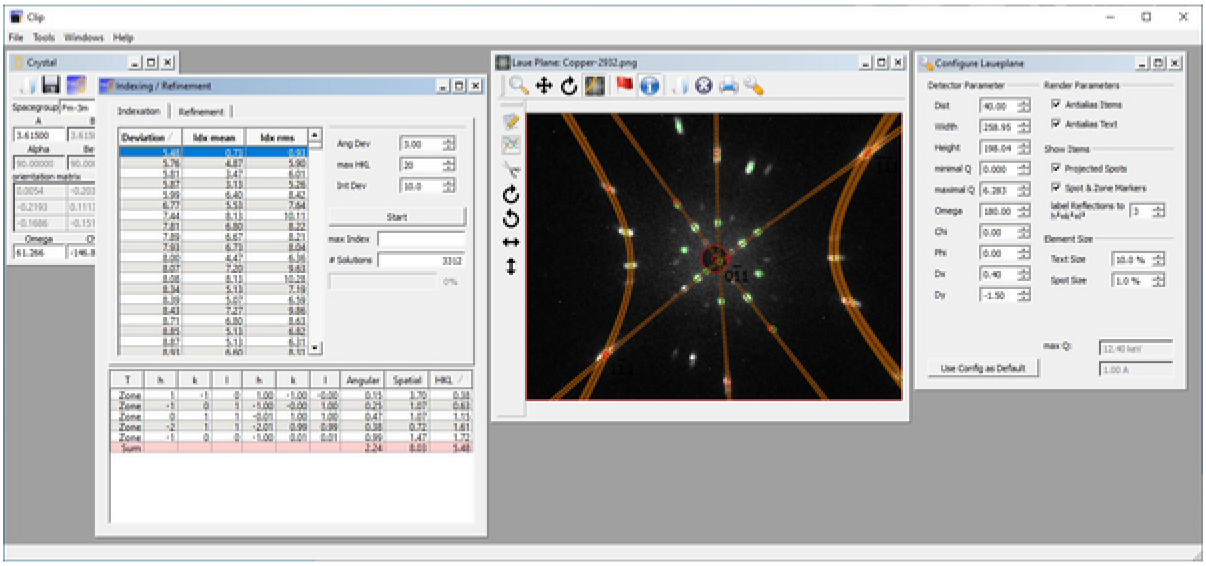
9. Choose the best indexation

CLIP will return a number of index options.

They may be sorted via their *Deviation* and/or their *Idx rms* , with smaller values being better matches.

Click on one of the options to see it displayed, and use the arrow keys to scroll through the options.

Don't forget to have the *Projected Spots* option toggled 'on' in the **Configure Laueplane** window.



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Reorientation: How far are you from perfect alignment?

Once the data have been successfully indexed, the **Tools: Reorientation** menu option will open the **Reorient** window.

This is very useful for determining how close the alignment is to perfect.

Enter the desired vector in the **Orient** field.

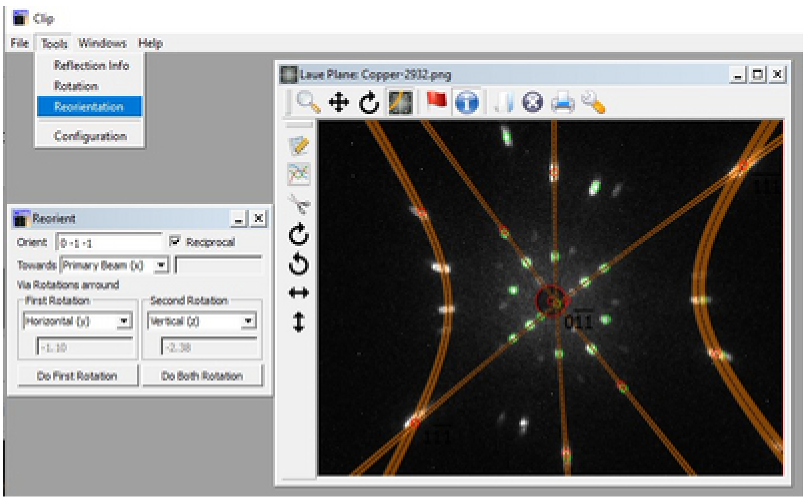
Use the checkbox immediately to the right to specify whether the vector is *real space* or *reciprocal space* .

Choose thd desired *direction* for the vector relative to the instrument in the **Towards** field.

Choose the rotation axes directions and the order for the rotations in the **Via rotations** fields

The rotation angles will appear below.

Having the *First rotation* around the *Horizontal (y)* axis is particulary useful (c.f. figure to the right), as this angle will show how far a desired scattering plane is from horizontal.



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Rotation: What happens if I rotate the crystal?

To have confidence that the indexing is correct, the crystal can be rotated by a set angle and another image can be measured.

CLIP can then be used to predict the position of the spots. Once the new spot positions are calculated, the new image can be loaded. If the indexing is correct, the predicted and measured spot positions will coincide.

The predicted spot positions can be calculated intuitively using the **Rotation** tool.

The **Tools: Rotation** menu option will open the **Rotation** window.

The rotation axis is selected from the drop menu at the top of the **Rotation** window. Note that:

the **Vertical (z)** axis is always the axis for the **omega** motor on OrientExpress.

the **Primary Beam (x)** axis points toward the reactor. This corresponds to the **tilt2** motor when **omega** = 0.

the **Horizontal (y)** axis points towards the Chartreuse mountain range (away from the IN16 guide). This corresponds to the **tilt1** motor when **omega** = 0.

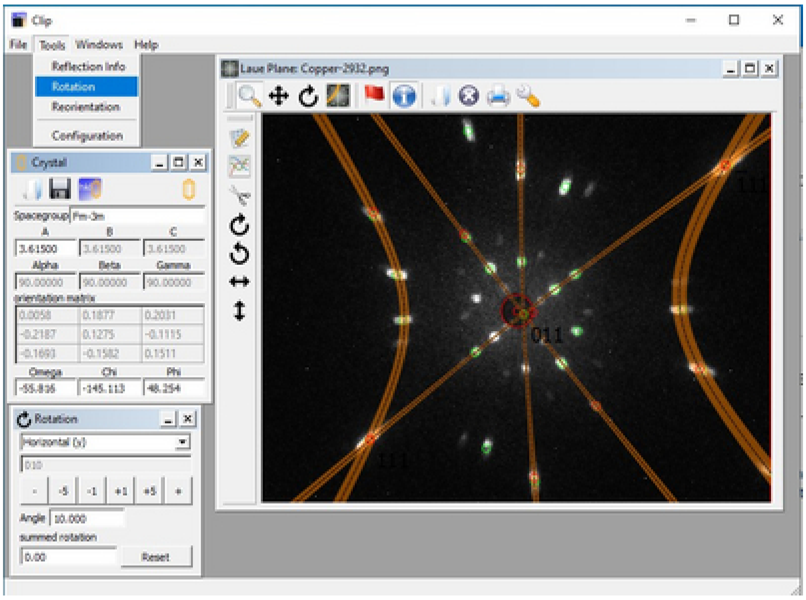
The rotation can be changed by set increments of ±1° or ±5° using the buttons.

The rotation can be changed by an arbitrary value by typing a number in the **Angle** field.

As an example:

1. Measure and index an image.
2. Rotate **omega** by +30° and collect another image.
3. Use the **Rotation** tool in CLIP to rotate the **Vertical (z)** axis by +30°.
4. Open the new image in CLIP. If the indexing is correct, the predicted and measured spots will coincide.

Note that similar rotations can be performed by changing the values in the **Omega**, **Chi**, and **Phi** fields of the **Crystal** window, however these correspond to Euler cradle angles. While the **Omega** angle corresponds to the **omega** motor on OrientExpress, **Chi**, and **Phi** do not correspond to the **tilt1** and **tilt2** motors.
The **Rotation** tool is a more intuitive method for calculating rotations as it allows for rotation about orthogonal axes.



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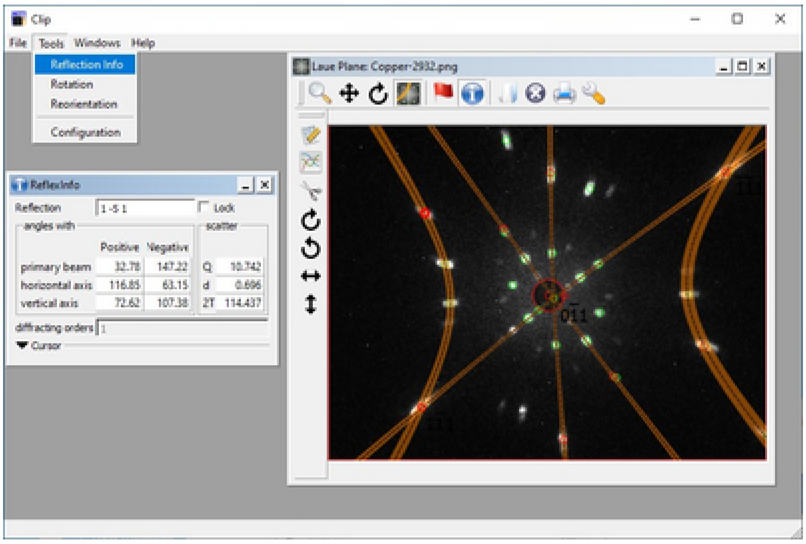
Reflection Info: Interrogating the indexed peaks

Once the data have been successfully indexed, the **Tools: Reflection Info** menu option will open the **ReflexInfo** window.

Clicking on peak positions will give information on the Miller indices, the momentum transfer and d-spacing, and the angles that the peak makes with respect to the important instrument axes.



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