Introduction to ORDER:
ORientation Definition Extending to Reciprocal space
Software for the PEAXIS instrument at Helmholtz Zentrum Berlin

Version 1.1
by Maciej Bartkowiak

Foreword

ORDER software was created as a tool for the users of the PEAXIS instrument at the Helmholtz Zentrum Berlin.

If you want to measure a powder/polycrystalline sample, or you never heard of a “UB matrix” before, then this software will not be of critical importance to you. **However, the .SAM sample definition files from ORDER can be loaded directly into CHaOS**, the PEAXIS instrument control software. If you want your sample information to be saved in the data files during the experiment, you can use ORDER to create the sample definition files. **Independent of how you create the .SAM files, you are encouraged to send them to the PEAXIS instrument scientists before the experiment.**

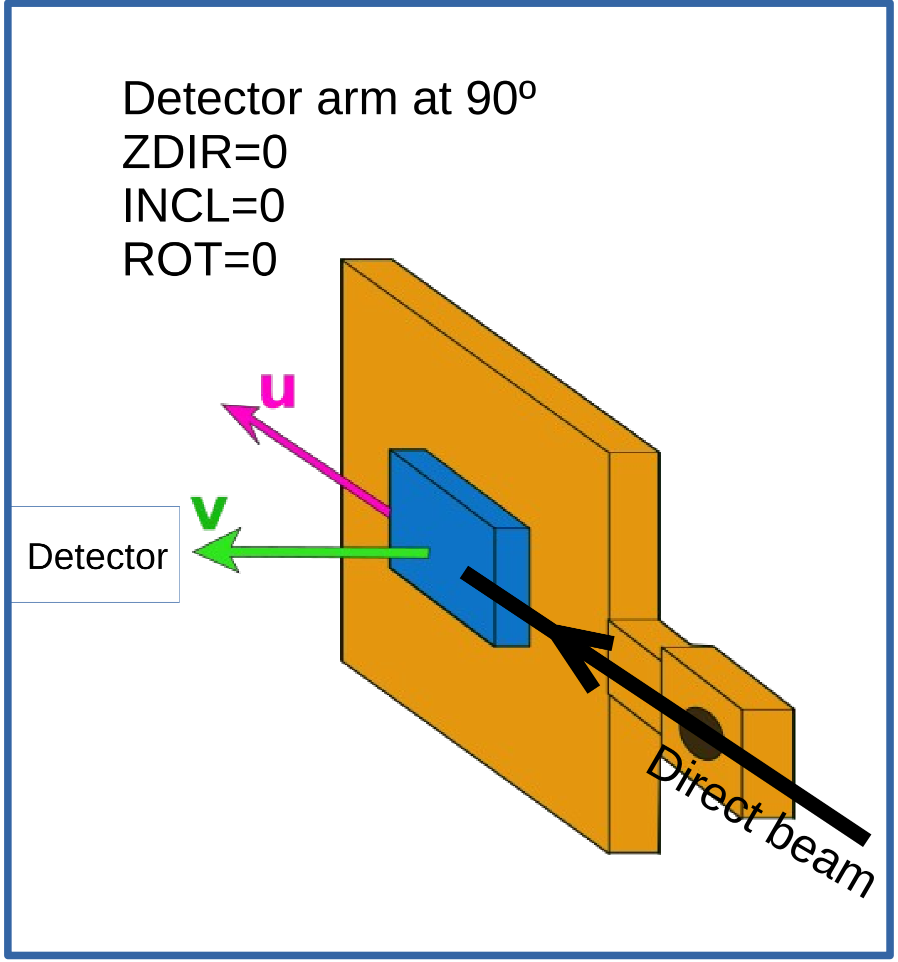
ORDER is written in Python and licensed under GNU GPL v3. This means that it is free software, and you are entitled (and encouraged) to download and read the source code of ORDER. If you re-use parts of this code in your own software and release the software to the users, you will have to make the source code available too.

Sample orientation on PEAXIS

The sample orientation on the PEAXIS instrument is largely preconditioned by the orientation on the sample holder itself.

The **u** and **v** vectors correspond to those defined by Busing and Levy in their paper:
Acta Crystallographica **22**, 457 (1967)
DOI: 10.1107/S0365110X67000970

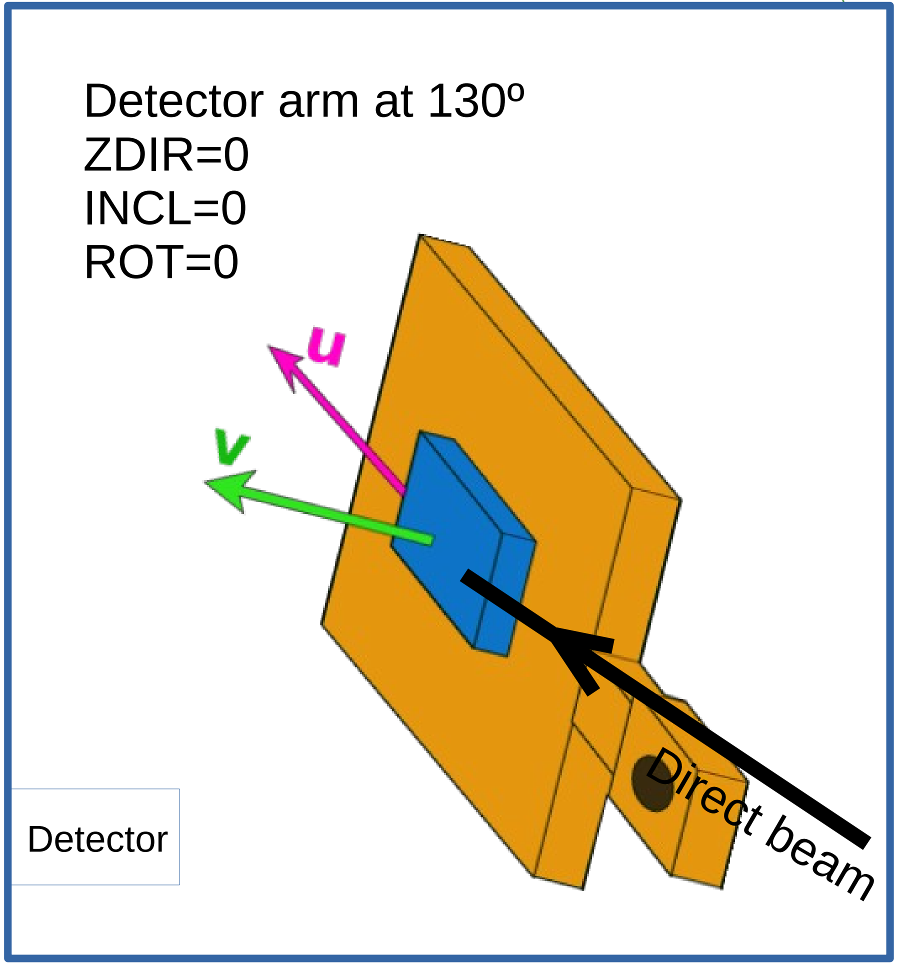
The **u** and **v** used by ORDER are identical to the Busing and Levy definition when the detector arm is at 90 degrees, and the 3 rotation angles of the manipulator are set to 0.



Sample orientation on PEAXIS

The entire sample chamber, including the manipulator, is tilted around the beam direction when the detector arm moved away from the 90º position. The tilt angle is a function of the detector arm position. If a specific sample orientation has to be maintained, the manipulator motors are used to compensate for the tilting.

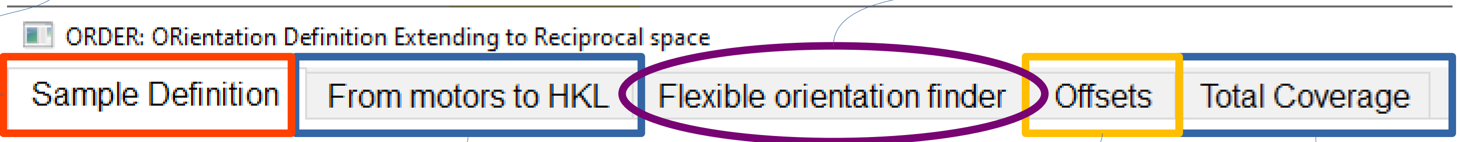
The main feature of ORDER is that it can tell the users how to reach a specific position in the reciprocal space, and it compensates for the chamber tilt at the same time.



The capabilities of ORDER.

Definition of the sample unit cell and orientation on the holder can be specified here. Critical for single-crystal samples.

The most important tab: it can calculate the motor positions of the instrument needed to create the desired scattering geometry. You can choose which parts of the geometry are fixed, depending on which parameters are important in your experiment.



This tab can take the instrument parameters and tell you where in the reciprocal space you are.

This tab can be used to correct the sample orientation by offsets based on the specular reflection position.

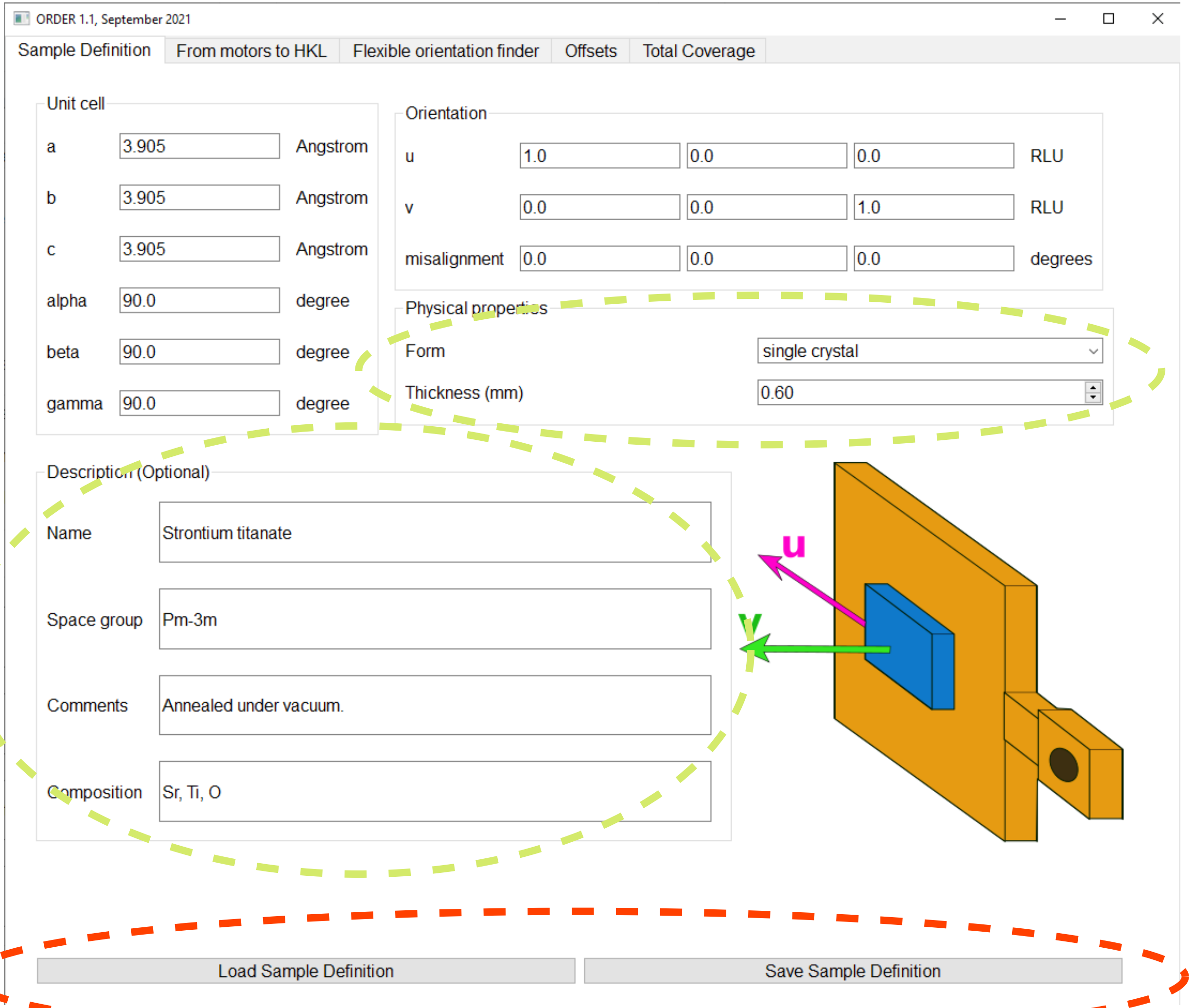
Shows the entire coverage of the instrument. Useful in the early stages of experiment planning, to check if your experiment is feasible.

Sample Definition

As the first step, it is necessary to define the crystallographic unit cell of the sample.

Information input here can be useful during the experiment, and makes the experiment documentation more complete.

Save your sample definition to a file. You can load it later, or share it with the instrument scientists.

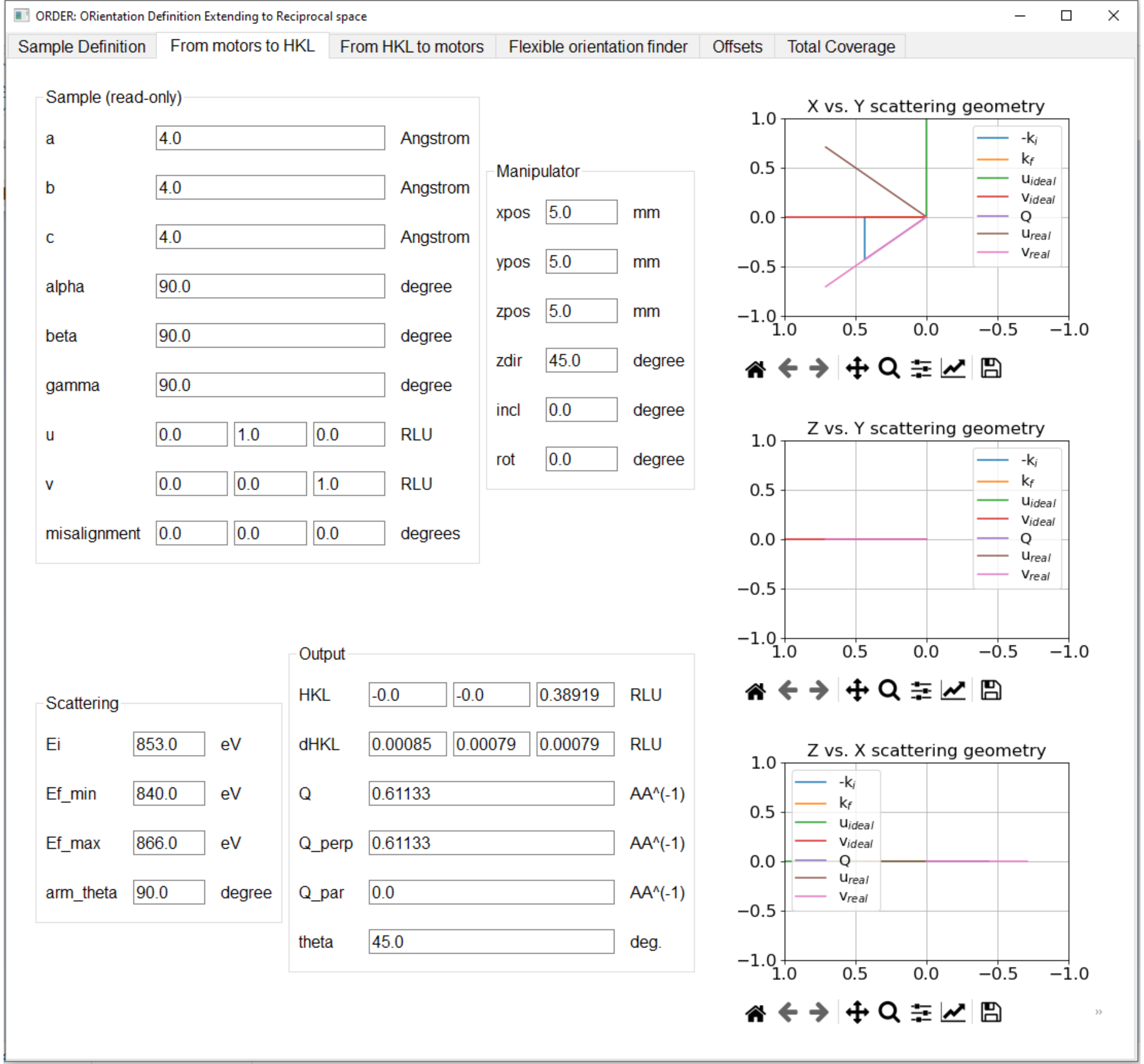


From motors to HKL

The input here consists of the manipulator motor positions, and the incoming photon energy.

Additionally, the sample definition is copied from the first tab.

The calculated output shows:
1. The current position in the reciprocal space,
2. The absolute value of the Q vector,
3. The angle **theta** between the incoming beam and the sample surface.



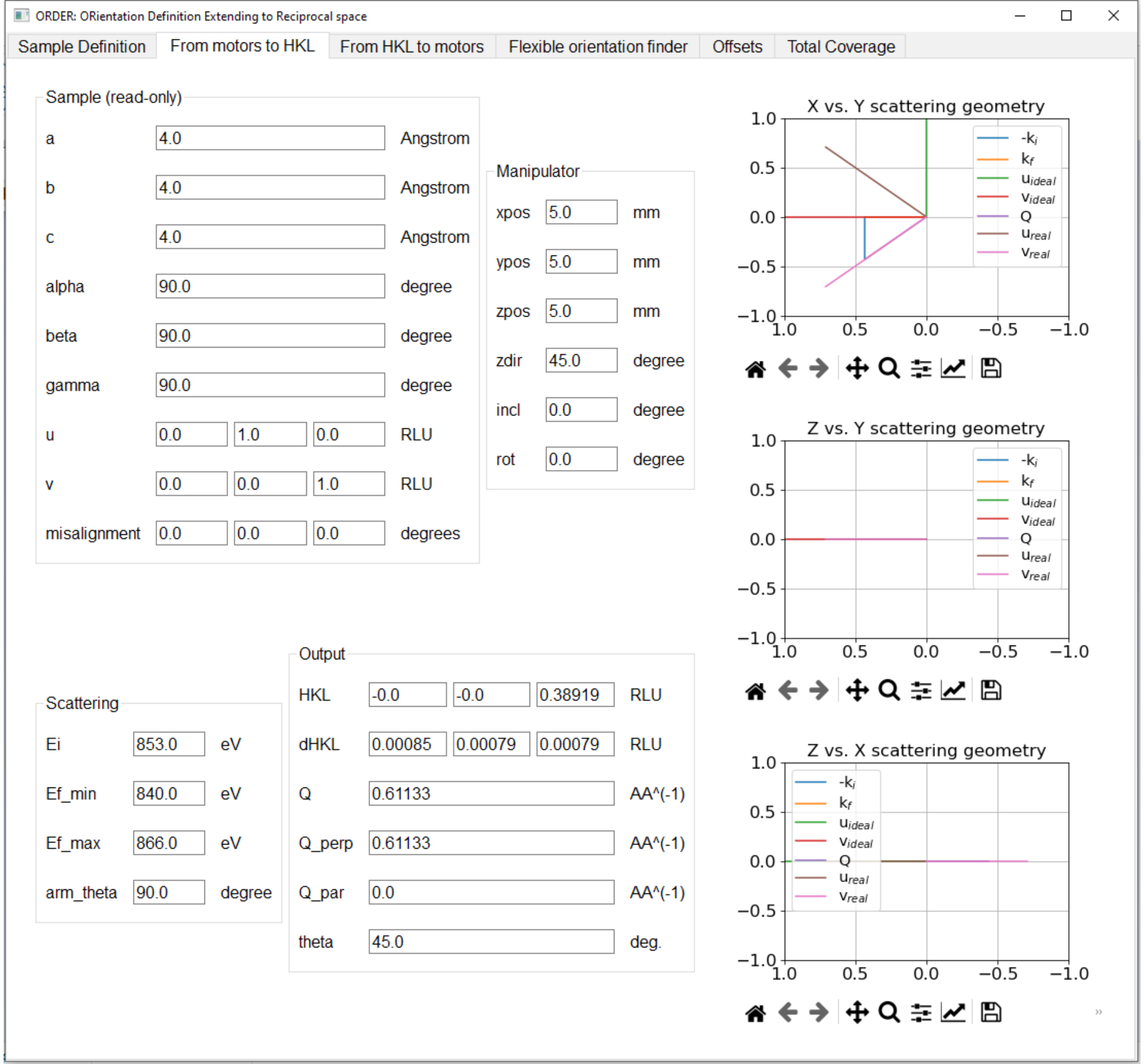
From motors to HKL

The scattering vector Q is also decomposed into two components, Q_perp and Q_par.

Q_perp is the component of Q that is perpendicular to the sample surface (i.e. the projection of Q onto the normal vector of the sample surface.)

Q_par is the component of Q in the sample surface plane.

$$Q^2 = Q\_par^2 + Q\_perp^2$$

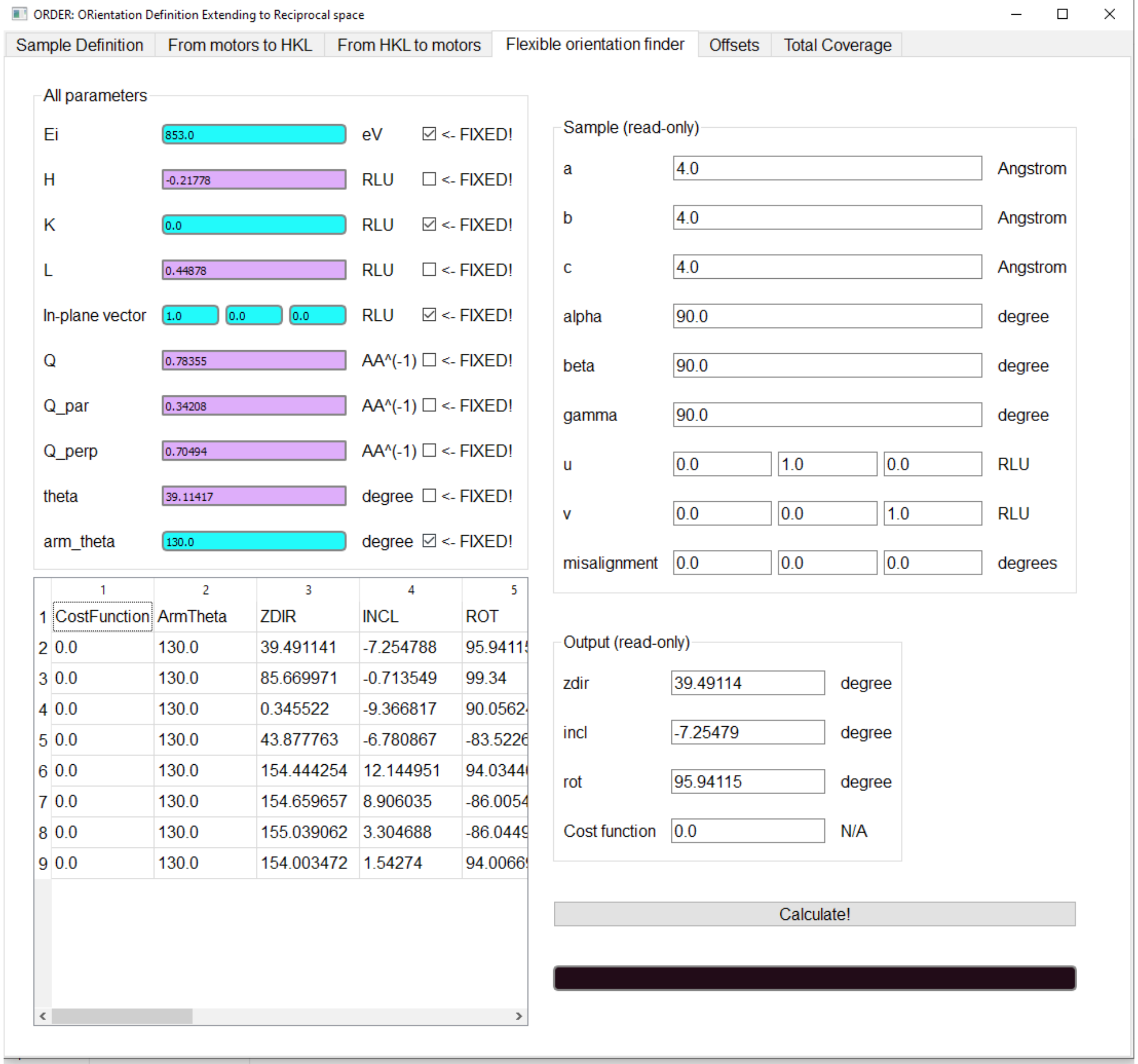


Flexible orientation finder

The FIXED parameters are those that must remain at the specified value. For example, if you want to use the 853 eV photon energy, keep it FIXED at that value.

The software will calculate the manipulator motor positions needed to reach the target.

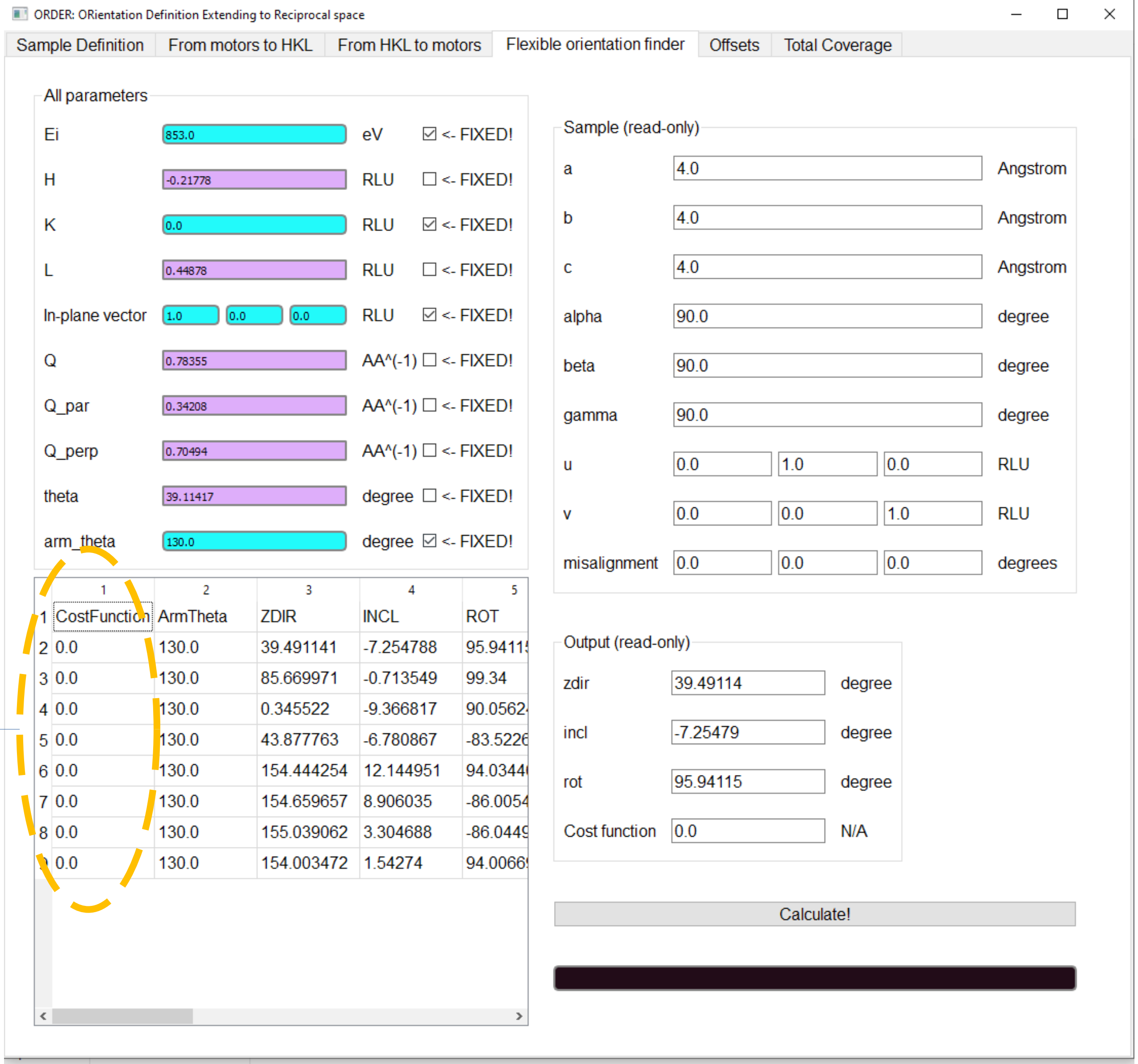
Only the solutions with CostFunction=0 are correct.



Flexible orientation finder

If the FIXED parameters are mutually exclusive, there will be no solution with CostFunction=0. It means that it is not possible to find a sample orientation that will satisfy all the requirements.

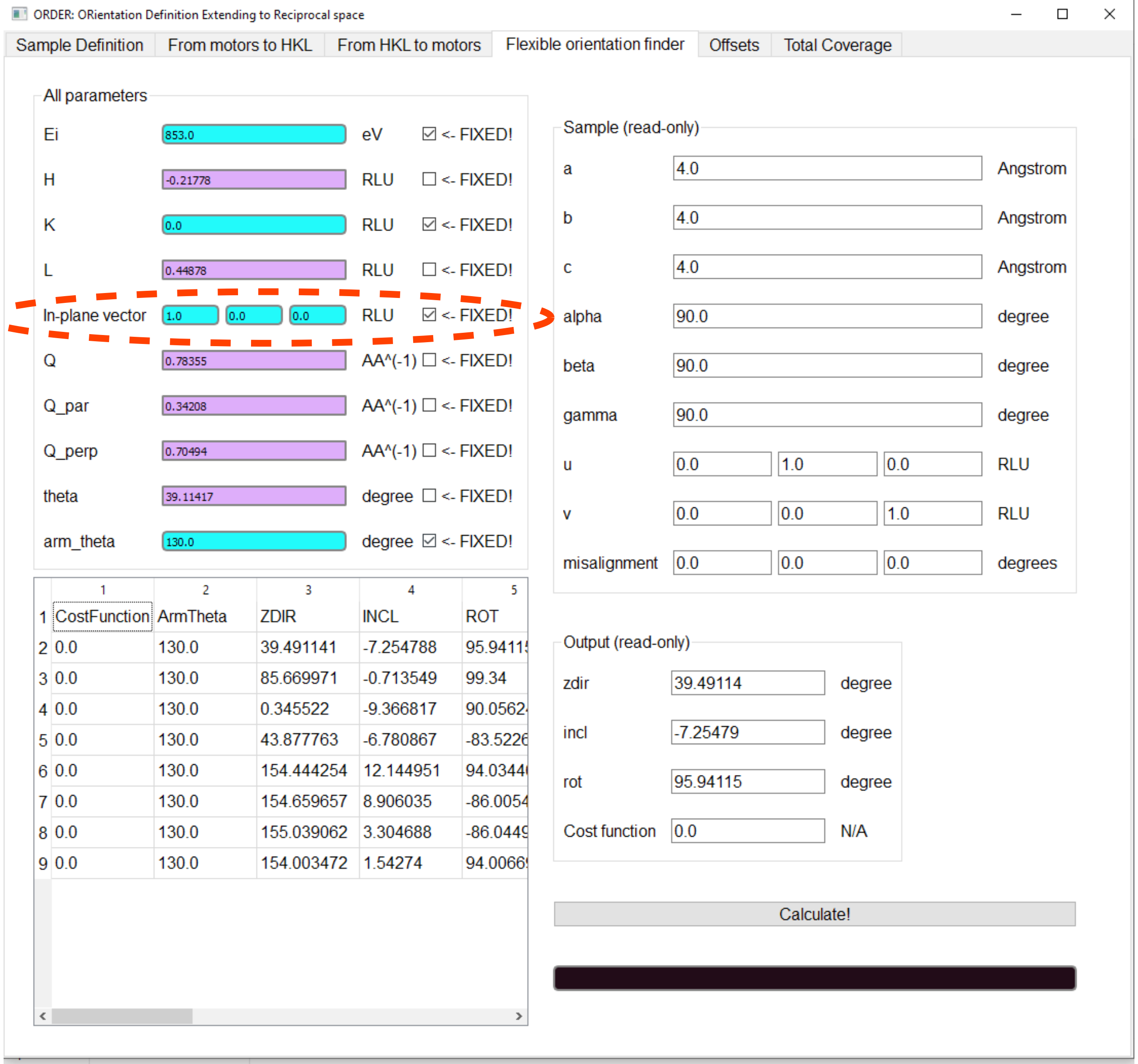
It is also possible to have many correct solutions. You can compare them, and pick the best one.



Flexible orientation finder

The “in-plane vector” is a reciprocal space vector that should be kept in the scattering plane of the instrument.

By keeping this vector fixed in your experiment, you can have the software compensate for the sample chamber tilt by applying a rotation around the **v** vector. Many users like to keep the **u** vector in the scattering plane.



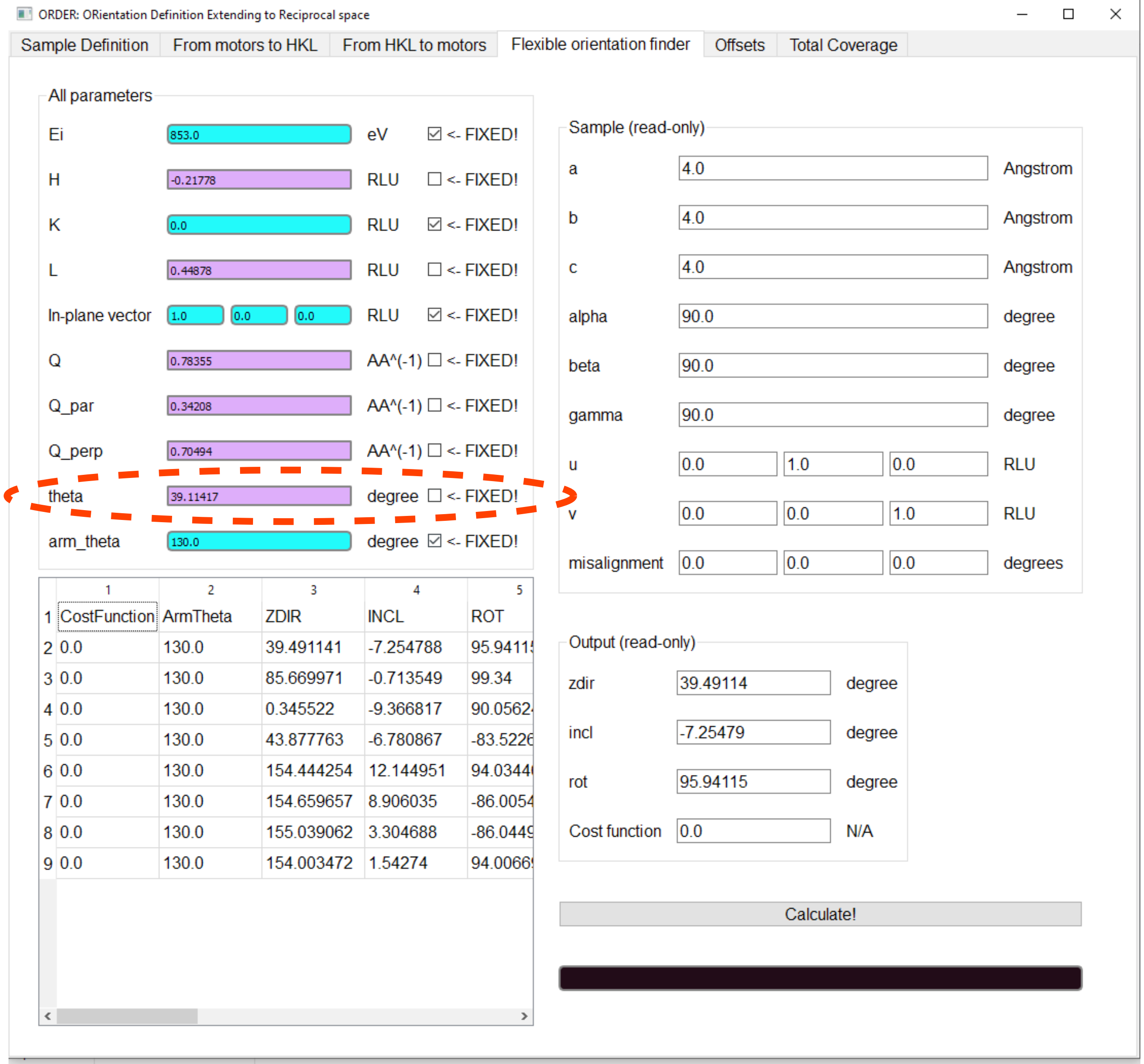
Flexible orientation finder

Theta is the angle between the incoming photon beam and the surface of the sample.

Theta=90º is normal incidence.

Theta=0º is (fully) grazing incidence.

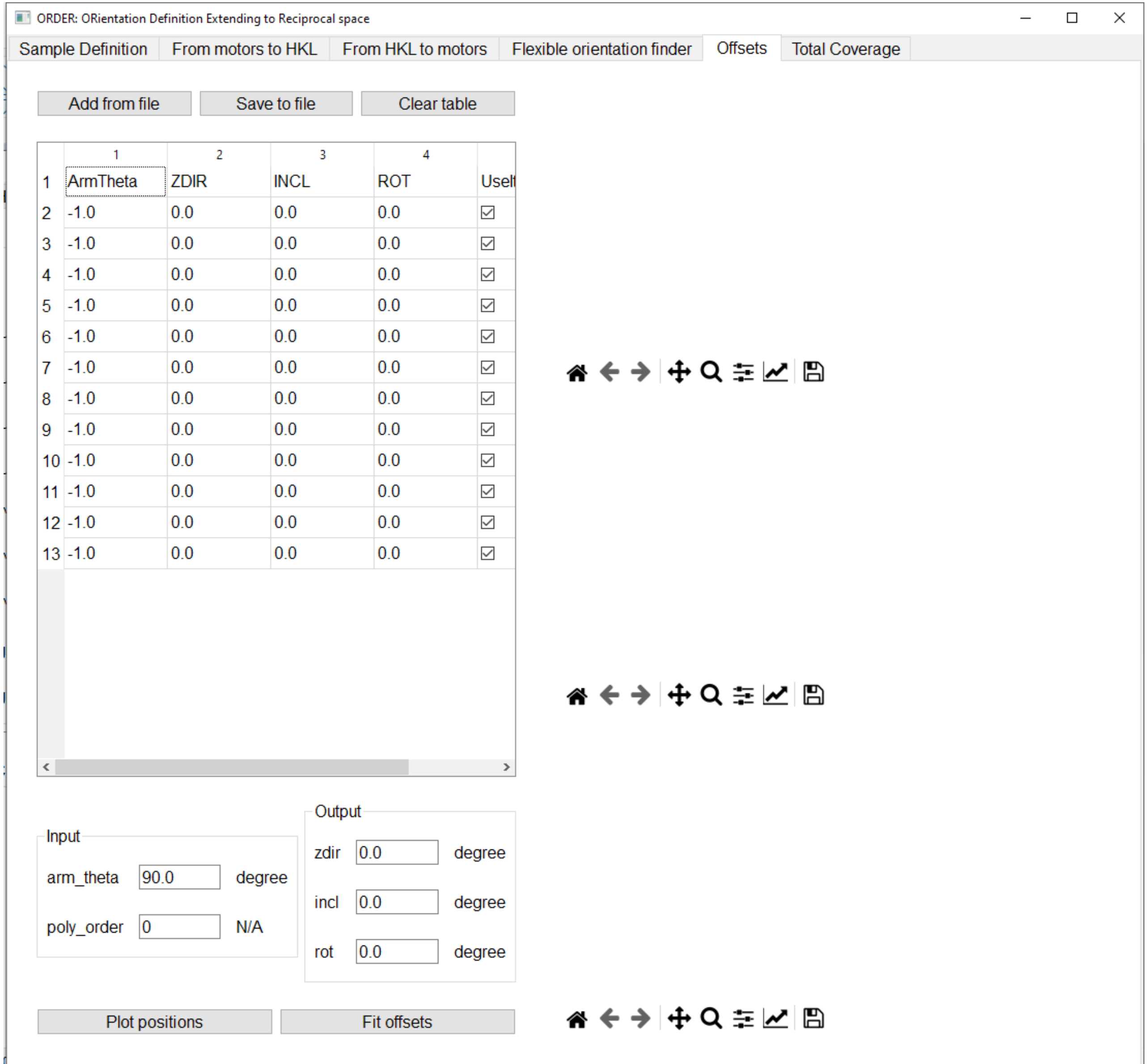
In a real-life experiment a non-zero value of theta is needed to observe signal in the detector.



Offsets

This tab can only be used once you have experimentally confirmed that the specular reflection is not exactly at the expected positon.

Once you have input some positions at which you found the real specular reflection, you can fit and extrapolate them to other detector arm angles, and predict the offsets needed to find it at those angles.



Total coverage

This tab calculates all the Q vector values that can be reached by PEAXIS for a specific photon energy. The different Q values are reached by moving the detector arm.

Some important K-edges (blue) and L-edges (red) are included in the plot.