

## ORDER



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

Version 1.0  
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## 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.

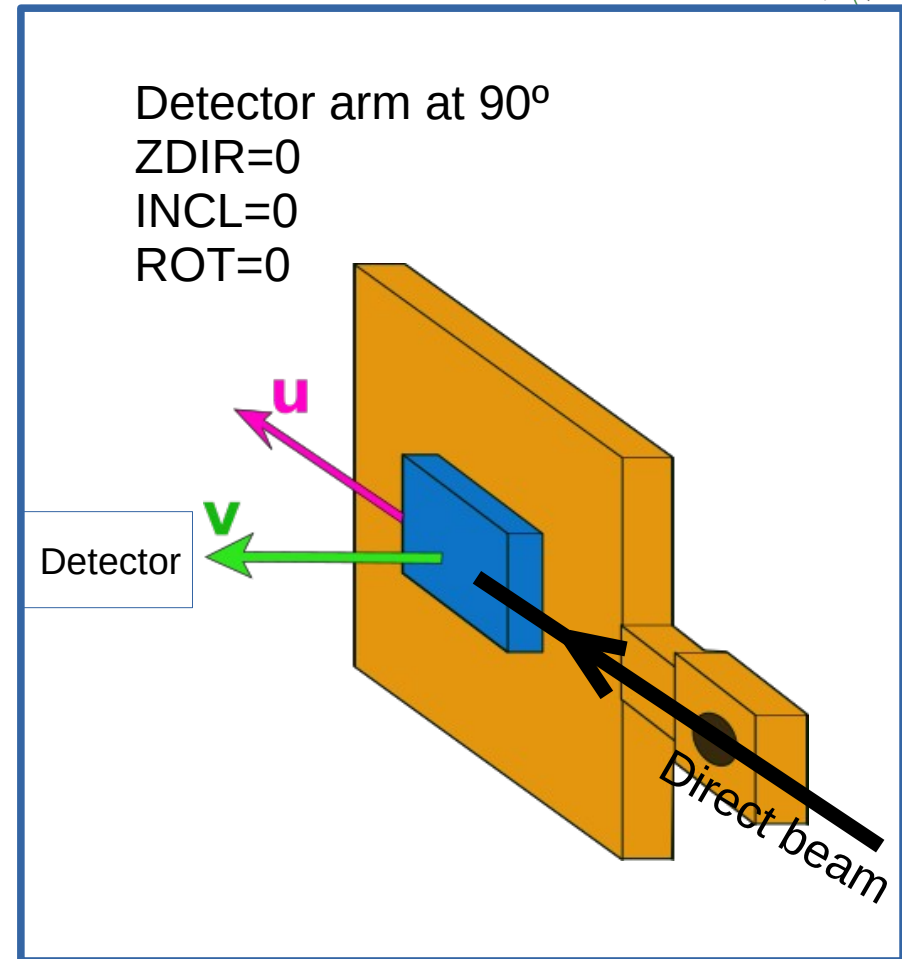
ORDER is written in Python and licensed under GNU GPL v3. This means that it is free software, and you are entitled (and encouraged) to download and read the source code of ORDER. If you re-use parts of this code in your own software and release the software to the users, you will have to make the source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

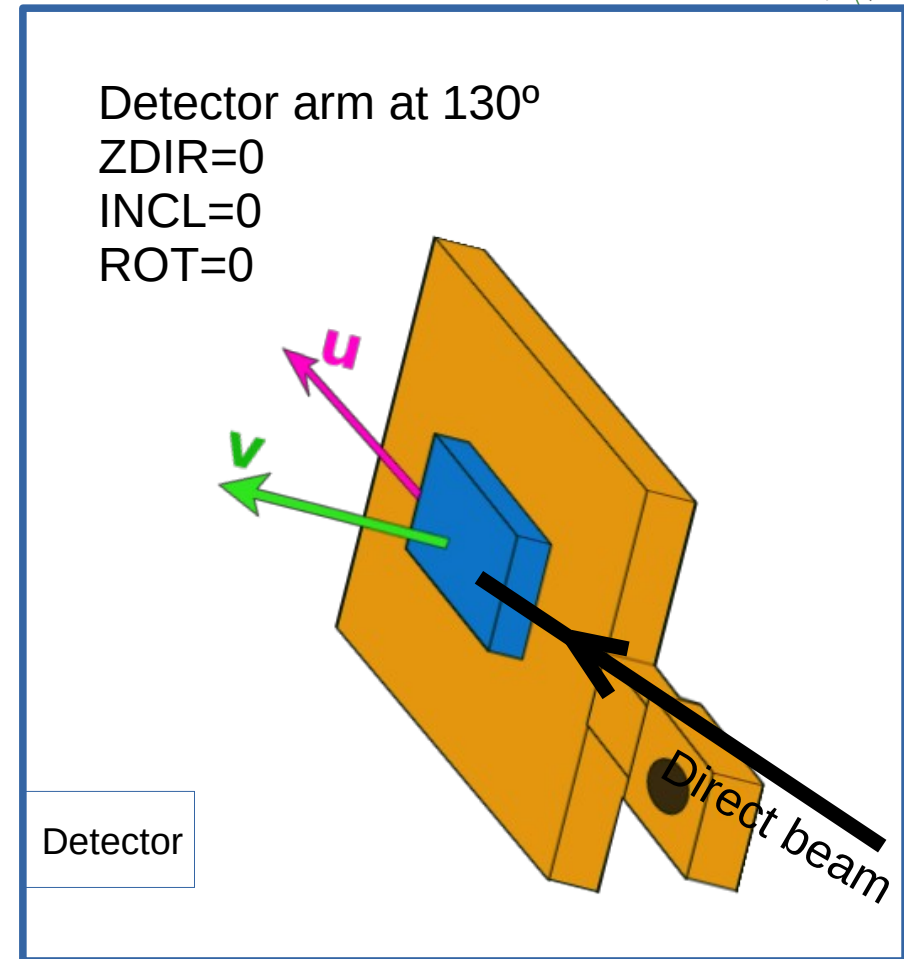
The **u** and **v** used by ORDER are identical to the Busing and Levy definition when the detector arm is at 90 degrees, and the 3 rotation angles of the manipulator are set to 0.



## 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 90° 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.

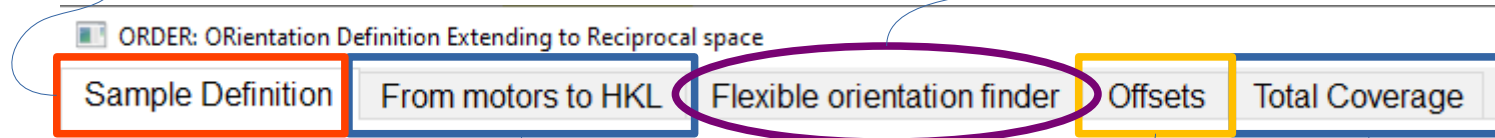
The main feature of ORDER is that it can tell the users how to reach a specific position in the reciprocal space, and it compensates for the chamber tilt at the same time.



## 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.

ORDER: Orientation Definition Extending to Reciprocal space

Sample Definition From motors to HKL Flexible orientation finder Offsets Total Coverage

Unit cell

a	<input type="text" value="4.0"/>	Angstrom
b	<input type="text" value="4.0"/>	Angstrom
c	<input type="text" value="4.0"/>	Angstrom
alpha	<input type="text" value="90.0"/>	degree
beta	<input type="text" value="90.0"/>	degree
gamma	<input type="text" value="90.0"/>	degree

Orientation

u	<input type="text" value="0.0"/>	<input type="text" value="1.0"/>	<input type="text" value="0.0"/>	RLU
v	<input type="text" value="0.0"/>	<input type="text" value="0.0"/>	<input type="text" value="1.0"/>	RLU
misalignment	<input type="text" value="0.0"/>	<input type="text" value="0.0"/>	<input type="text" value="0.0"/>	degrees

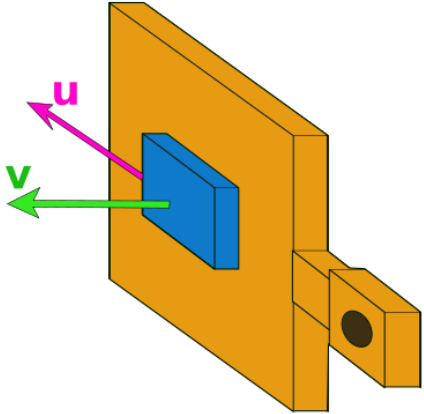
Description (Optional)


Name

Formula

Space group

Comments



ORDER 

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.

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ORDER: Orientation Definition Extending to Reciprocal space

Sample Definition From motors to HKL From HKL to motors Flexible orientation finder Offsets Total Coverage

Sample (read-only)

a	4.0	Angstrom		
b	4.0	Angstrom		
c	4.0	Angstrom		
alpha	90.0	degree		
beta	90.0	degree		
gamma	90.0	degree		
u	0.0	1.0	0.0	RLU
v	0.0	0.0	1.0	RLU
misalignment	0.0	0.0	0.0	degrees

Manipulator

xpos	5.0	mm
ypos	5.0	mm
zpos	5.0	mm
zdir	45.0	degree
incl	0.0	degree
rot	0.0	degree

Scattering

Ei	853.0	eV
Ef_min	840.0	eV
Ef_max	866.0	eV
arm_theta	90.0	degree

Output

HKL	-0.0	-0.0	0.38919	RLU
dHKL	0.00085	0.00079	0.00079	RLU
Q	0.61133			AA <sup>(-1)</sup>
Q_perp	0.61133			AA <sup>(-1)</sup>
Q_par	0.0			AA <sup>(-1)</sup>
theta	45.0			deg.

X vs. Y scattering geometry

Z vs. Y scattering geometry

Z vs. X scattering geometry

# From motors to HKL

The scattering vector  $Q$  is also decomposed into two components,  $Q_{\text{perp}}$  and  $Q_{\text{par}}$ .

$Q_{\text{perp}}$  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.)

$Q_{\text{par}}$  is the component of  $Q$  in the sample surface plane.

$$Q^2 = Q_{\text{par}}^2 + Q_{\text{perp}}^2$$

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ORDER: Orientation Definition Extending to Reciprocal space

Sample Definition From motors to HKL From HKL to motors Flexible orientation finder Offsets Total Coverage

Sample (read-only)

a  Angstrom

b  Angstrom

c  Angstrom

alpha  degree

beta  degree

gamma  degree

u    RLU

v    RLU

misalignment    degrees

Manipulator

xpos  mm

ypos  mm

zpos  mm

zdir  degree

incl  degree

rot  degree

Scattering

Ei  eV

Ef\_min  eV

Ef\_max  eV

arm\_theta  degree

Output

HKL    RLU

dHKL    RLU

Q  AA<sup>(-1)</sup>

Q\_perp  AA<sup>(-1)</sup>

Q\_par  AA<sup>(-1)</sup>

theta  deg.

X vs. Y scattering geometry

Z vs. Y scattering geometry

Z vs. X scattering geometry



# 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.

ORDER: ORIENTATION DEFINITION EXTENDING TO RECIPROCAL SPACE

Sample Definition | From motors to HKL | From HKL to motors | Flexible orientation finder | Offsets | Total Coverage

All parameters

Ei	853.0	eV	<input checked="" type="checkbox"/> <- FIXED!
H	-0.21778	RLU	<input type="checkbox"/> <- FIXED!
K	0.0	RLU	<input checked="" type="checkbox"/> <- FIXED!
L	0.44878	RLU	<input type="checkbox"/> <- FIXED!
In-plane vector	1.0 0.0 0.0	RLU	<input checked="" type="checkbox"/> <- FIXED!
Q	0.78355	AA <sup>(-1)</sup>	<input type="checkbox"/> <- FIXED!
Q_par	0.34208	AA <sup>(-1)</sup>	<input type="checkbox"/> <- FIXED!
Q_perp	0.70494	AA <sup>(-1)</sup>	<input type="checkbox"/> <- FIXED!
theta	39.11417	degree	<input type="checkbox"/> <- FIXED!
arm_theta	130.0	degree	<input checked="" type="checkbox"/> <- FIXED!

	1	2	3	4	5
1	CostFunction	ArmTheta	ZDIR	INCL	ROT
2	0.0	130.0	39.491141	-7.254788	95.941115
3	0.0	130.0	85.669971	-0.713549	99.34
4	0.0	130.0	0.345522	-9.366817	90.0562
5	0.0	130.0	43.877763	-6.780867	-83.5226
6	0.0	130.0	154.444254	12.144951	94.0344
7	0.0	130.0	154.659657	8.906035	-86.0054
8	0.0	130.0	155.039062	3.304688	-86.0449
9	0.0	130.0	154.003472	1.54274	94.0066

Sample (read-only)

a	4.0	Angstrom
b	4.0	Angstrom
c	4.0	Angstrom
alpha	90.0	degree
beta	90.0	degree
gamma	90.0	degree
u	0.0 1.0 0.0	RLU
v	0.0 0.0 1.0	RLU
misalignment	0.0 0.0 0.0	degrees

Output (read-only)

zdir	39.49114	degree
incl	-7.25479	degree
rot	95.94115	degree
Cost function	0.0	N/A

Calculate!

# 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.

Sample Definition From motors to HKL From HKL to motors Flexible orientation finder Offsets Total Coverage

All parameters

Ei 853.0 eV  <- FIXED!

H -0.21778 RLU  <- FIXED!

K 0.0 RLU  <- FIXED!

L 0.44878 RLU  <- FIXED!

In-plane vector 1.0 0.0 0.0 RLU  <- FIXED!

Q 0.78355 AA<sup>(-1)</sup>  <- FIXED!

Q\_par 0.34208 AA<sup>(-1)</sup>  <- FIXED!

Q\_perp 0.70494 AA<sup>(-1)</sup>  <- FIXED!

theta 39.11417 degree  <- FIXED!

arm\_theta 130.0 degree  <- FIXED!

	1	2	3	4	5
1 CostFunction		ArmTheta	ZDIR	INCL	ROT
2 0.0	130.0	39.491141	-7.254788	95.941115	
3 0.0	130.0	85.669971	-0.713549	99.34	
4 0.0	130.0	0.345522	-9.366817	90.0562	
5 0.0	130.0	43.877763	-6.780867	-83.5226	
6 0.0	130.0	154.444254	12.144951	94.0344	
7 0.0	130.0	154.659657	8.906035	-86.0054	
8 0.0	130.0	155.039062	3.304688	-86.0449	
0.0	130.0	154.003472	1.54274	94.0066	

Sample (read-only)

a 4.0 Angstrom

b 4.0 Angstrom

c 4.0 Angstrom

alpha 90.0 degree

beta 90.0 degree

gamma 90.0 degree

u 0.0 1.0 0.0 RLU

v 0.0 0.0 1.0 RLU

misalignment 0.0 0.0 0.0 degrees

Output (read-only)

zdir 39.49114 degree

incl -7.25479 degree

rot 95.94115 degree

Cost function 0.0 N/A

Calculate!

# 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.

Sample Definition From motors to HKL From HKL to motors Flexible orientation finder Offsets Total Coverage

All parameters

Ei	853.0	eV	<input checked="" type="checkbox"/>	<- FIXED!
H	-0.21778	RLU	<input type="checkbox"/>	<- FIXED!
K	0.0	RLU	<input checked="" type="checkbox"/>	<- FIXED!
L	0.44878	RLU	<input type="checkbox"/>	<- FIXED!
In-plane vector	1.0 0.0 0.0	RLU	<input checked="" type="checkbox"/>	<- FIXED!
Q	0.78355	AA <sup>(-1)</sup>	<input type="checkbox"/>	<- FIXED!
Q_par	0.34208	AA <sup>(-1)</sup>	<input type="checkbox"/>	<- FIXED!
Q_perp	0.70494	AA <sup>(-1)</sup>	<input type="checkbox"/>	<- FIXED!
theta	39.11417	degree	<input type="checkbox"/>	<- FIXED!
arm_theta	130.0	degree	<input checked="" type="checkbox"/>	<- FIXED!

Sample (read-only)

a	4.0	Angstrom
b	4.0	Angstrom
c	4.0	Angstrom
alpha	90.0	degree
beta	90.0	degree
gamma	90.0	degree
u	0.0 1.0 0.0	RLU
v	0.0 0.0 1.0	RLU
misalignment	0.0 0.0 0.0	degrees

Output (read-only)

zdir	39.49114	degree
incl	-7.25479	degree
rot	95.94115	degree
Cost function	0.0	N/A

Calculate!

	1	2	3	4	5
1	CostFunction	ArmTheta	ZDIR	INCL	ROT
2	0.0	130.0	39.491141	-7.254788	95.941115
3	0.0	130.0	85.669971	-0.713549	99.34
4	0.0	130.0	0.345522	-9.366817	90.0562
5	0.0	130.0	43.877763	-6.780867	-83.5226
6	0.0	130.0	154.444254	12.144951	94.0344
7	0.0	130.0	154.659657	8.906035	-86.0054
8	0.0	130.0	155.039062	3.304688	-86.0449
9	0.0	130.0	154.003472	1.54274	94.0066

# Flexible orientation finder

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

Theta=90° is normal incidence.

Theta=0° is (fully) grazing incidence.

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

Sample Definition From motors to HKL From HKL to motors Flexible orientation finder Offsets Total Coverage

All parameters

Ei 853.0 eV  <- FIXED!

H -0.21778 RLU  <- FIXED!

K 0.0 RLU  <- FIXED!

L 0.44878 RLU  <- FIXED!

In-plane vector 1.0 0.0 0.0 RLU  <- FIXED!

Q 0.78355 AA<sup>(-1)</sup>  <- FIXED!

Q\_par 0.34208 AA<sup>(-1)</sup>  <- FIXED!

Q\_perp 0.70494 AA<sup>(-1)</sup>  <- FIXED!

theta 39.11417 degree  <- FIXED!

arm\_theta 130.0 degree  <- FIXED!

Sample (read-only)

a 4.0 Angstrom

b 4.0 Angstrom

c 4.0 Angstrom

alpha 90.0 degree

beta 90.0 degree

gamma 90.0 degree

u 0.0 1.0 0.0 RLU

v 0.0 0.0 1.0 RLU

misalignment 0.0 0.0 0.0 degrees

Output (read-only)

zdir 39.49114 degree

incl -7.25479 degree

rot 95.94115 degree

Cost function 0.0 N/A

Calculate!

	1	2	3	4	5
1	CostFunction	ArmTheta	ZDIR	INCL	ROT
2	0.0	130.0	39.491141	-7.254788	95.941115
3	0.0	130.0	85.669971	-0.713549	99.34
4	0.0	130.0	0.345522	-9.366817	90.0562
5	0.0	130.0	43.877763	-6.780867	-83.5226
6	0.0	130.0	154.444254	12.144951	94.0344
7	0.0	130.0	154.659657	8.906035	-86.0054
8	0.0	130.0	155.039062	3.304688	-86.0449
9	0.0	130.0	154.003472	1.54274	94.0066

# Offsets

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

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.

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ORDER: Orientation Definition Extending to Reciprocal space

Sample Definition From motors to HKL From HKL to motors Flexible orientation finder Offsets Total Coverage

Add from file Save to file Clear table

	1	2	3	4	Use
1	ArmTheta	ZDIR	INCL	ROT	Use
2	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
3	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
4	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
5	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
6	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
7	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
8	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
9	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
10	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
11	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
12	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>
13	-1.0	0.0	0.0	0.0	<input checked="" type="checkbox"/>

Input

arm\_theta  degree

poly\_order  N/A

Output

zdir  degree

incl  degree

rot  degree

Plot positions Fit offsets

# 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.

