



Introduction to ORDER:

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

> Version 1.1 by Maciej Bartkowiak

27/09/21

**ORDER User Guide - PEAXIS Instrument** 

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.

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.



ORDEF

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.



ORDER

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.

ORDER: ORientation Definition Extending to Reciprocal space

From motors to HKL Flexible orientation finder Sample Definition

Offsets Total Coverage

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.

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# 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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mple Definition	From motors to	HKL Fro	m HKL to motors	Flex	ible orientati	ion finder	Offsets	Total Coverag	е		
Sample (read-	only)							X vs. Y so	attering	geometry	
а	4.0		Angstrom				1.0				]
				Manip	oulator		0.5			K <sub>f</sub>	-
b	4.0		Angstrom	XDOS	5.0	mm	0.0		$\searrow$	Videal	
С	4.0		Angstrom				0.0			ureal	
alpha	90.0		degree	ypos	5.0	mm	-0.5			·ieai	
				zpos	5.0	mm	-1.0				
beta	90.0		degree	zdir	45.0	dearee	1	.0 0.5	0.0	-0.5	1.0
gamma	90.0		degree	2011		degree		€⇒.₩.	く キ 🖉	: B	
	0.0 1.0	0.0	RU	incl	0.0	degree		Z vs. Y so	attering	geometry	
u		0.0		rot	0.0	degree	1.0				]
v	0.0	1.0	RLU				0.5			k <sub>f</sub> u <sub>ideal</sub>	
misalignment	0.0 0.0	0.0	degrees				0.0			Videal	
										ureal Vreal	
							-0.5				
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Scattering		TINC	-0.0		0.00010	NEO		••••			
Ei 8	53.0 eV	dHKL	0.00085 0.00	079	0.00079	RLU	1.0	Z vs. X so	attering	geometry	٦
Ef_min 84	40.0 eV	Q	0.61133			AA^(-1)					
Ef_max 80	66.0 eV	Q_perp	0.61133			AA^(-1)	0.5	Uideal Videal			
arm theta	) 0 degree	O par	0.0			۵۵۸( 1)	0.0	Q — U <sub>rea</sub> /			-
	degree	⊲_pai	0.0			(v~ (- i)	-0.5				-
		theta	45.0			deg.	-1.0				
							1	.0 0.5	0.0	-0.5 -3	1.0

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# 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.

 $Q^2 = Q_par^2 + Q_perp^2$ 

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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.

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ĸ	DER: Orientation D	efinition Extending	to Reciprocal spac	e				
n	ple Definition	From motors	s to HKL Fro	om HKL	to moto	ors Fle	xible	orientation find
A	All parameters -							
E	Ei	853.0		eV	☑ <- [	FIXED!		Sample (read-
F	4	.0 21778		DIII				a
'		-0.21776		NLU	_	INLD!		b
k	< C	0.0		RLU	⊻ <-	FIXED!		U
L		0.44878		RLU	□<-	FIXED!		С
lr	n-plane vector	1.0 0.0	0.0	RLU	⊻ <-	FIXED!		alpha
C	2	0.78355		AA^(-1)	) 🗆 <- F	FIXED!		beta
C	Q_par	0.34208		AA^(-1)	) 🗆 <- F	FIXED!		gamma
C	2_perp	0.70494		AA^(-1)	) 🗆 <- F	FIXED!		
tł	heta	39.11417		degree	□ <-	FIXED!		ŭ
9	urm theta	130.0		dogroo				v
ů	ann_incia	(155.5		ucgree				misalignment
	1	2	3	4	L.	5		
	CostFunction	Armineta			70.0	RUI		Output (read o
2	0.0	130.0	39.491141	-1.2541	88	95.9411		Output (read-o
3	0.0	130.0	85.669971	-0.7135	549	99.34		zdir
4	0.0	130.0	0.345522	-9.3668	317	90.0562		inal
5	0.0	130.0	43.877763	-6.7808	367	-83.5226		IIICI
3	0.0	130.0	154.444254	12.144	951	94.0344		rot
7	0.0	130.0	154.659657	8.9060	35	-86.0054		
3	0.0	130.0	155.039062	3.3046	88	-86.0449		Cost function
9	0.0	130.0	154.003472	1.5427	4	94.0066		

IUI	e onentation int	Unsets	iotai C	overage		
	-Sample (read-	only)				
	a	4.0				Angstrom
	b	4.0				Angstrom
	с	4.0				Angstrom
	alpha	90.0				degree
	beta	90.0				degree
	gamma	90.0				degree
	u	0.0	1.0	0.0	0	RLU
	v	0.0	0.0	1.0	0	RLU
	misalignment	0.0	0.0	0.0	0	degrees
	Output (read-o	nly)				
	zdir	39.49114		degree		
	incl	-7.25479		degree		
	rot	95.94115		degree		
	Cost function	0.0		N/A		

Calculate!

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         53.0         eV         <<         FIXEDI         a         4.0           H         0.21775         RLU         <<         FIXEDI         a         4.0           K         0.0         RLU         <<         FIXEDI         b         4.0           L         0.44978         RLU         <<         FIXEDI         c         4.0           In-plane vector         L0         0.0         0.0         RLU         <<         FIXEDI         alpha         90.0           Q_par         0.34905         AA^(1)         <         FIXEDI         alpha         90.0         0           gamma         90.0	Angstrom
All parameters         Ei $83.0$ $eV$ $\leq$ - FIXEDI         H $0.2172$ RLU $<$ - FIXEDI         K $0.0$ RLU $\leq$ - FIXEDI         L $0.44878$ RLU $\leq$ - FIXEDI         In-plane vector $10$ $0.0$ $0.0$ Q $0.78355$ $AA^{(-1)}$ $<$ - FIXEDI         Q_par $0.34208$ $AA^{(-1)}$ $<$ - FIXEDI         u $0.0$ $1.0$ $0.0$ $0perp$ $0.70494$ $AA^{(-1)}$ $<$ - FIXEDI         u $0.0$ $1.0$ $0.0$ $1$ $2$ $3$ $4$ $5$ $1$ $2$ $3$ $4$ $5$ $1$ $2$ $3$ $4$ $5$ $1$ $2$ $3$ $4$ $5$ $1$ $2$ $3$ $4$ $5$ $10$ $0.0$ $0.0$ $0.0$ $0.0$ $1$ $2$ $3$ $4$ $5$ $10$ $130.0$ $34949114$	Angstrom
Ei       853.0 $eV$ $\leq <$ FIXED!       Sample (read-only)         H $0.21778$ RLU $< <$ FIXED!       a $4.0$ K $0.0$ RLU $< <$ FIXED!       b $4.0$ L $0.44878$ RLU $< <$ FIXED!       c $4.0$ L $0.44878$ RLU $< <$ FIXED!       c $4.0$ Q $0.78355$ $AA^{n}(-1)$ $< <$ FIXED!       alpha $90.0$ Q_par $0.34208$ $AA^{n}(-1)$ $< <$ FIXED!       beta $90.0$ Q_perp $0.7944$ $AA^{n}(-1)$ $< <$ FIXED! $u$ $0.0$ $1.0$ arm theta $39.11417$ degree $< <$ FIXED! $u$ $0.0$ $0.0$ $1.0$ $1$ $2$ $3$ $4$ $5$ $v$ $0.0$ $0.0$ $1.0$ $1$ $2$ $3$ $4$ $5$ $v$ $0.0$ $0.0$ $0.0$ $2$ $0.0$ $130.0$ $39.491141$ $.7.254788$ $95.94112$ $v$ $0.0$ $0.0$	Angstrom Angstrom
H $0.21773$ RLU $< FIXED!$ a $4.0$ K $0.0$ RLU $< < FIXED!$ b $4.0$ L $0.44878$ RLU $< < FIXED!$ c $4.0$ In-plane vector $1.0$ $0.0$ $0.0$ RLU $< < FIXED!$ alpha $90.0$ Q $0.78355$ $AA^{1}(-1)$ $< < FIXED!$ $alpha$ $90.0$ Q_par $0.34208$ $AA^{1}(-1)$ $< < FIXED!$ $beta$ $90.0$ Q_perp $0.70994$ $AA^{1}(-1)$ $< < FIXED!$ $u$ $0.0$ $1.0$ arm_theta $39.11417$ $degree$ $< < FIXED!$ $u$ $0.0$ $1.0$ $v$ 1       2       3       4 $5$ $v$ $0.0$ $0.0$ $0.0$ 2 $0.0$ $130.0$ $39.491141$ $7.254788$ $95.9411$ $v$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ $0.0$ <	Angstrom
K       0.0       RLU       ☑ < FIXED!       b       4.0         L       0.44973       RLU       □ < FIXED!	Angstrom
L $0.44878$ RLU $< < FIXED!$ c $4.0$ In-plane vector       10 $0.0$ $0.0$ RLU $\leq < FIXED!$ $alpha$ $90.0$ Q $0.78355$ $AA^{(-1)}$ $< < FIXED!$ $beta$ $90.0$ Q_par $0.34208$ $AA^{(-1)}$ $< < FIXED!$ $beta$ $90.0$ Q_perp $0.20494$ $AA^{(-1)}$ $< < FIXED!$ $u$ $0.0$ $1.0$ $0.0$ theta $39.11417$ degree $< < FIXED!$ $u$ $0.0$ $1.0$ $0.0$ $1$ $2$ $3$ $4$ $5$ $rv 0.0 0.0 0.0 1 2 3 4 5 rv 0.0 0.0 0.0 1 2 3 4 5 rv 0.0 0.0 0.0 1 2 3 4 5 rv 0.0 0.0 0.0 2 0.0 130.0 3.4477763 6.780867 83.5226$	
In-plane vector       10       0.0       0.0       RLU $\leq <$ FIXED!       alpha       90.0         Q       0.78335       AA^(-1) $\leq <$ FIXED!       beta       90.0         Q_par       0.34208       AA^(-1) $\leq <$ FIXED!       gamma       90.0         Q_perp       0.70494       AA^(-1) $\leq <$ FIXED!       u       0.0       1.0       0.0         theta       39.11417       degree $< <$ FIXED!       u       0.0       1.0       0.0         arm_theta       10.0       39.491141 $.7.254788$ 95.94115       0.0       0.0       0.0       0.0         2       0.0       130.0       85.669971 $.0.713549$ 99.34       0.0       130.0       345522 $.9.366817$ 90.0562       0.0       10 $.7.25479$ degree         5       0.0       130.0       154.459657       8.906035       .80.056       60.056       10       95.94115       degree         rot       95.94115       degree $.7.25479$ degree       10 $.7.25479$ degree	Angstrom
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	degree
Q_par       0.34208       AA^(-1) □ <- FIXED!	degree
Q_perp $0.70494$ $AA^{(-1)} \square <-FIXED!$ theta $39.11417$ degree $\square <-FIXED!$ arm_theta $130.0$ degree $\square <-FIXED!$ $1$ $2$ $3$ $1$ $2$ $3$ $1$ $2$ $3$ $1$ $2$ $3$ $1$ $2$ $3$ $2$ $0.0$ $130.0$ $30.0$ $130.0$ $39.491141$ $7.254788$ $95.94115$ $0.0$ $130.0$ $33.45522$ $9.366817$ $90.0562$ $5$ $0.0$ $130.0$ $130.0$ $43.877763$ $6.780867$ $6$ $0.0$ $130.0$ $154.444254$ $12.144951$ $94.03444$ $7$ $0.0$ $154.659657$ $7$ $0.0$ $130.0$ $154.659657$	degree
theta $39.11417$ degree $\square < FIXED!$ arm_theta $130.0$ degree $\square < FIXED!$ $1$ $\square 2$ $3$ $4$ $\square 5$ $1$ $\square costFunction ArmTheta ZDIR INCL ROT 2 0.0 130.0 39.491141 -7.254788 95.941113$ $0.0$ $130.0$ $85.669971$ $-0.713549$ $99.344$ $0.0$ $130.0$ $0.345522$ $-9.366817$ $90.05625$ $0.0$ $130.0$ $43.877763$ $-6.780867$ $-83.52266$ $0.0$ $130.0$ $154.444254$ $12.144951$ $94.034417$ $0.0$ $130.0$ $154.444254$ $12.144951$ $94.034417$ $0.0$ $130.0$ $154.659657$ $8.006035$ $86.0054$	RLU
arm_theta       130.0       degree ⊠ <- FIXED!	RLU
1       2       3       4       5         1       CostFunction       ArmTheta       ZDIR       INCL       ROT         2       0.0       130.0       39.491141       -7.254788       95.94119         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       154.659657       8.906035       .86.0054	degrees
CostFunction       ArmTheta       ZDIR       INCL       ROT         2       0.0       130.0       39.491141       -7.254788       95.94114         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	
2       0.0       130.0       39.491141       -7.254788       95.94113       Output (read-only)         3       0.0       130.0       85.669971       -0.713549       99.34       zdir       39.491141       degree         4       0.0       130.0       0.345522       -9.366817       90.0562       incl       -7.25479       degree         5       0.0       130.0       154.444254       12.144951       94.03444       rot       95.94115       degree         7       0.0       130.0       154.659657       8.06035       .86.0054       80.054	
3       0.0       130.0       85.669971       -0.713549       99.34       zdir       39.49114       degree         4       0.0       130.0       0.345522       -9.366817       90.0562       incl       -7.25479       degree         5       0.0       130.0       154.444254       12.144951       94.0344       other       -7.25479       degree         6       0.0       130.0       154.659657       8.906035       .86.0054       86.0054       95.94115       degree	
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	
5       0.0       130.0       43.877763       -6.780867       -83.5226       incl       -7.25479       degree         6       0.0       130.0       154.444254       12.144951       94.0344       rot       95.94115       degree	
6 0.0 130.0 154.444254 12.144951 94.0344 rot 95.94115 degree	
7 0 0 130 0 154 659657 8 906035 86 0054	
100.0 104.000001 0.000000 -00.0000	
8 0.0 130.0 155.039062 3.304688 -86.0449 Cost function 0.0 N/A	
0.0 130.0 154.003472 1.54274 94.0066	
Calculate!	

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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.

			111.21		Els: 1		den orr	1 T ( )	0	
ample Definition	From moto	ors to HKL F	rom HKL	to motors	Flexi	ble orientation fin	der Offs	ets Total	Coverage	
- All parameters										
- 						-Sample (read	-only)			
	853.0		ev		Di		10			<b>A</b>
Н	-0.21778		RLU	□ <- FIXE	D!	а	4.0			Angstrom
к	0.0		RLU	⊠ <- FIXF	וס	b	4.0			Angstrom
L	0.44878		RLU	□ <- FIXE	D!	С	4.0			Angstrom
In-plane vector	1.0 0.0	0.0	RLU	☑ <- FIXE	D!	alpha	90.0			degree
	_									
Q	0.78355		AA^(-1	) 🗆 <- FIXE	:D!	beta	90.0			degree
Q_par	0.34208		AA^(-1	) 🗆 <- FIXE	D!	gamma	90.0			degree
Q perp	0.70494		AA^(-1	) □ <- FIXF	וח					
d <sup>-b</sup> oth				,		u	0.0	1.0	0.0	RLU
theta	39.11417		degree □ <- FIXED!			v	0.0	0.0	1.0	RLU
arm_theta	130.0		degree	e	D!					
	1					misalignment	0.0	0.0	0.0	degrees
1 1 CostEunction	2 ArmTheta		INCL	PO.	5 T					
2 0 0	130.0	39 491141	-7 254	788 95.0	94114	Output (read-o	only)			
3 0 0	130.0	85 669971	-0.713	549 99 (	34	adie	20 4011		dograa	
4 0.0	130.0	0.345522	-9.366	817 90.0	0562	Zuli	39.49114	•	degree	
5 0.0	130.0	43.877763	-6.780	867 -83	5226	incl	-7.25479		degree	
6 0.0	130.0	154.444254	12.144	951 94.0	0344	rot	05 04445	:	dograe	
7 0.0	130.0	154.659657	8.9060	35 -86	0054	TOL	95.94113	)	degree	
8 0.0	130.0	155.039062	3.3046	88 -86	0449	Cost function	0.0		N/A	
9 0.0	130.0	154.003472	1.5427	4 94.0	0066					
								Calcu	ate!	
<					>					

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**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.

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

Sample Definition	From moto	rs to HKL Fi	rom HKL	to mot	ors F	lexib	le orientation find	der	Offsets	Total (	Covera	ge	
All parameters													
Ei	853.0		eV	<-	FIXED!	!	Sample (read-	only)					
н	-0.21778		RLU	□ <-	FIXED!	!	а	4.0					Angstrom
к	0.0		RLU	✓ <-	FIXED!	!	b	4.0					Angstrom
L	0.44878		RLU	_ <-	FIXED!	!	с	4.0					Angstrom
In-plane vector	1.0 0.0	0.0	RLU	<-	FIXED!	!	alpha	90.0	)				degree
Q	0.78355		AA^(-1	) 🗆 <-	FIXED!	!	beta	90.0	)				degree
Q_par	0.34208		AA^(-1	) 🗆 <-	FIXED!	!	gamma	90.0	)				degree
Q_perp	0.70494		AA^(-1	) 🗆 <-	FIXED!	!	u	0.0		1.0		0.0	RLU
theta	39.11417		degree	e 🗆 <-	FIXED!		>	0.0		0.0		10	RIII
arm_theta	130.0		degree	e ⊠ <-	FIXED!	!	v	0.0		0.0			
1	2	3		4		5	misalignment	0.0		0.0		0.0	degrees
1 CostFunction	ArmTheta	ZDIR	INCL		ROT								
2 0.0	130.0	39.491141	-7.254	788	95.941	11:	Output (read-o	only)-					
3 0.0	130.0	85.669971	-0.713	549	99.34		zdir	39.4	9114		dear	ee	
4 0.0	130.0	0.345522	-9.366	817	90.056	52·							
5 0.0	130.0	43.877763	-6.780	867	-83.52	26	incl	-7.2	5479		degr	ee	
6 0.0	130.0	154.444254	12.144	4951	94.034	14(		05.0					
7 0.0	130.0	154.659657	8.9060	035	-86.00	54	rot	95.9	94115		aegr	ee	
8 0.0	130.0	155.039062	3.3046	588	-86.04	49	Cost function	0.0			N/A		
9 0.0	130.0	154.003472	1.5427	74	94.006	66!							
										Calcula	ate!		
<						>							

ORDER: ORientation Definition Extending to Reciprocal space

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# 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.

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4	-1.0	0.0	0.0	0.0	$\checkmark$			
5	-1.0	0.0	0.0	0.0	$\checkmark$			
6	-1.0	0.0	0.0	0.0	$\checkmark$			
7	-1.0	0.0	0.0	0.0	$\checkmark$	<b>☆ ← →</b> ⊕ Q 幸 ∠ 🖺		
8	-1.0	0.0	0.0	0.0	$\checkmark$			
9	-1.0	0.0	0.0	0.0	$\checkmark$			
10	-1.0	0.0	0.0	0.0	$\checkmark$			
11	-1.0	0.0	0.0	0.0	$\checkmark$			
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27/09/21

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#### 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.

