Direct Geometry Alignment Script Documentation

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# Purpose of the script

This script can be used for calculating the UB matrix for Single Crystal diffraction data, and for giving the UB with a specific peak aligned to beam direction. Currently written for MERLIN, MAPS, LET but can be extended in future, refer to Appendix 3 for further information.

Contents

[Section 1: User inputs 3](#_Toc207360089)

[1.1: Lattice Parameters 3](#_Toc207360090)

[1.2 Data Input 3](#_Toc207360091)

[1.3 UB Calculation and Orientation 4](#_Toc207360092)

[1.4: Peak Prediction 5](#_Toc207360093)

[Section 2: Staff Inputs 7](#_Toc207360094)

[2.1 File handling 7](#_Toc207360095)

[2.2 Data analysis inputs 7](#_Toc207360096)

[Section 3: Peak picking methods 8](#_Toc207360097)

[3.1 Manual 8](#_Toc207360098)

[3.2 ROI Method 9](#_Toc207360099)

[Section 4: Calculate UB methods 11](#_Toc207360100)

[ONE\_PEAK 11](#_Toc207360101)

[TWO\_PEAKS 11](#_Toc207360102)

[THREE\_PEAKS 11](#_Toc207360103)

[FIVEPLUS\_PEAKS 11](#_Toc207360104)

[Section 5: Reorientation 12](#_Toc207360105)

[5.1 Psi Rotation 12](#_Toc207360106)

[5.2 Phi Rotation 12](#_Toc207360107)

[Section 6 Verification Methods 13](#_Toc207360108)

[6.1 Peak Prediction & Use 13](#_Toc207360109)

[Appendix 1: Text File Output 14](#_Toc207360110)

[Appendix 2: Class Definitions File 15](#_Toc207360111)

[Appendix 3: Adding Additional Instruments 16](#_Toc207360112)

[Appendix 4: List of Space Groups 17](#_Toc207360113)

# Section 1: User inputs

## 1.1: Lattice Parameters

lattice\_parameters = {

"a": ,  
"b": ,  
"c": ,  
"alpha": ,  
"beta": ,  
"gamma":

}

}

This block defines the lattice parameters for the sample.

* Enter the lattice parameters (in Angstroms) and angles (in degrees). Example:

lattice\_parameters = {

"a": 5.43,  
"b": 5.39,  
"c": 20.5,  
"alpha": 60,  
"beta": 80,  
"gamma":90

}

## 1.2 Data Input

This section takes the run numbers of the data, peaks to be used, and the methods used to calculate the UB matrix of the sample.

run\_numbers = [""] #input as a list  
  
corresponding\_hkls = [] # please write in same order the runs are written in  
# e.g[[h1,k1,l1],[h2,k2,l2]]  
  
peak\_picking\_method = #Peak\_picking\_methods.{METHOD} e.g Peak\_picking\_methods.MANUAL

* run\_numbers: Input Run Numbers as a list, with each number closed by “” to declare the datatype correctly. If a run has multiple peaks it needs to be listed the corresponding number of times. Example: [“54017”, “54017”, “54016”]
* corresponding\_hkls: Enter the Miller indices of each peak to be used in the alignment, with each hkl being in the format of [[h1,k1,l1],[h2,k2,l2]]. The inputted hkls must be listed in the same order as the run numbers in which they are found. Example: [[2,0,0], [1,0,1],[0,0,4]] Per the example above, [2,0,0] and [1,0,1] must be found in Run 54017 and [0,0,4] in Run 54016.
* peak\_picking\_method is for choosing the method used by the script to get the peaks. Allowed options: MANUAL, ROI. For further details see Section 3: Peak picking methods

## 1.3 UB Calculation and Orientation

UB\_method = #UB\_METHOD.{CHOSEN\_METHOD} E.G UB\_METHOD.ONE\_PEAK Available methods:ONE\_PEAK, TWO\_PEAKS, THREE\_PEAKS, FIVEPLUS\_PEAKS  
  
#ONE\_PEAK = Method for known scattering plane + 1 peak  
#TWO\_PEAK = Method for if you are able to index 2 non-collinear peaks  
#THREE\_PEAK = 3 Peaks, lattice parameters are not required  
# this method compromises by minimising square differences between qs & ql  
#FIVEPLUS\_PEAKS = First automatically index peaks + find UB algorithm  
#for method = ONE PEAK, vectors defining the scattering plane are required  
vector\_1 = []  
vector\_2 = []  
  
# Peak to Orient to u vector  
Reorient = #Enter True or False  
hkl\_of\_desired\_alignment= [,] # please input as a single peak: [h,k,l]

This section takes inputs to define the method that will be used to calculate the UB matrix and a preferred orientation.

* UB\_method: Enter the method that will be used to calculate the alignment, in the format UB\_METHOD.{CHOSEN\_METHOD}. Example: UB.METHOD.ONE\_PEAK. For more details about calculate UB Methods refer to Section 4.
* vector\_1 and vector\_2: These are two vectors that define the scattering plane of the sample. They are given as hkl values and must not be collinear. They are only used for UB.METHOD.ONE\_PEAK. Example: [1,1,0] and [1,-1,0].]
* Reorient: Flag for whether the user would like UB rotated to have a provided peak aligned to beam direction
* hkl\_of\_desired\_alignment: this is the peak that the user would like aligned to the beam direction (u vector) for Psi=0. The angle required for the rotation is given in degrees, in the range [-180,180], where < 0 is clockwise, > 0 is anticlockwise.

## 1.4: Peak Prediction

This section allows for the calculated UB matrix to be used to predict the position of different peaks in order to verify the accuracy of the calculated UB matrix.

Predict\_peaks = #Enter true or false  
min\_dspacing =  
max\_dspacing =

unit\_cell\_space\_group = #this either needs to be a string of the symbol e.g "F d -3 m" or and integer with no "",  
# if you don't know your space group number enter "N/A"

unit\_cell\_symmetry = reflection\_condition.PRIMITIVE

#Use from available list and enter in the format reflection\_condition.{CELL\_SYMMETRY}, PRIMITIVE by default change by replacing PRIMITIVE with desired symmetry condition

* Predict\_peaks: True or False, whether the user would like this to be done after calculating the UB matrix.
* Unit\_cell\_space\_group is where the space group/number can be entered into this field, the Appendix contains a list of all allowed space group symbols. Symbols must be entered as a string e.g “F d -3 m”, or as a number e.g 65
* min\_dspacing & max\_dspacing are to mark the min and max d-spacing of the peaks that will be displayed. The values are given in inverse Angstroms and min\_dspacing must be less than max\_dspacing.
* unit\_cell\_symmetry gives the symmetry conditions to remove disallowed peaks from the prediction. Replace PRIMITIVE with desired symmetry from allowed list below or leave as PRIMITIVE to show all peaks.
* The PredictedPeaks workspace will be overlayed on the first run in the list

PRIMITIVE = "Primitive"  
 BODY\_CENTERED= "Body Centered"  
 C\_FACE\_CENTERED = "C-face centered"  
 B\_FACE\_CENTERED = "B-face centered"  
 A\_FACE\_CENTERED = "A-face centered"  
 ALL\_FACE\_CENTERED = "All-face centered"  
 RHOMBO\_CENTERED\_REV = "Rhombohedrally centred reverse"  
 HEX\_CENTERED\_REV = "Hexagonally centred, reverse"

Example:

Predict\_peaks = True #Enter true or false  
min\_dspacing = 1.5  
max\_dspacing = 6.0

unit\_cell\_space\_group = “C m m m” #this either needs to be a string of the symbol e.g "F d -3 m" or and integer with no "",  
# if you don't know your space group number return "N/A"

unit\_cell\_symmetry = reflection\_condition.PRIMITIVE

#Use from available list and enter in the format reflection\_condition.{CELL\_SYMMETRY}, PRIMITIVE by default change by replacing PRIMITIVE with desired symmetry condition

# Section 2: Staff Inputs

## 2.1 File handling

This section takes information about the instrument, cycle and RB for the data being collected to find the correct datafiles.

instrument\_name = #Enter instrument name in all caps  
cycle = “”  
rbnum = “”

* instrument\_name – name of the instrument. Currently supports the following options: MAPS, MERLIN, LET
* cycle: The cycle in which the data was collected, in the format “year\_number”. Example: “2025\_1”
* rbnum: The RB Number assigned to user’s experiment; data is stored in a folder with this number.

Example:

instrument\_name = MAPS #Enter instrument name in all caps  
cycle = “2025\_1”  
rbnum = “2510458”

## 2.2 Data analysis inputs

This section takes inputs for determining the tolerance parameters for the UB matrix determination and peak prediction.

d\_tolerance = #peaks\_radius in A^-1  
hkl\_tolerance =   
beam\_mode = #Return beam\_modes.{} e.g beam\_modes.WHITE\_BEAM possible modes: WHITE\_BEAM, MONOCHROMATIC

* d\_tolerance: The tolerance for d-spacing when adding peaks for the refinement. The value is given in inverse Angstroms and must be positive
* hkl\_tolerance: The tolerance in the Miller indices when indexing peaks during peak prediction. A single, positive value (in r.l.u.) is given, which applies to each hkl index.
* beam\_mode: Used to define if the runs measured were monochromatic or white beam mode. Possible values for this field are beam\_modes.WHITE\_BEAM or beam\_modes.MONOCHROMATIC.

# Section 3: Peak picking methods

## 3.1 Manual

The Instrument View interface will open for each of the instances of a run number in the list. Use the pick peak tool to choose your peak in Instrument view.

|  |  |
| --- | --- |
| a | b |
| c | d |

Figure 1 – Instrument viewer in Manual Mode

Steps to choose Manual Peak:

* If required, zoom in to the appropriate peak using the Zoom tool (see Fig. 1a). The peak being chosen is in the order listed in the script, with the current peak printed in the Mantid Messages panel.
* Select the Add Single Crystal Peak tool as shown in Fig. 1a.
* Click the peak on the Instrument View as shown in Fig. 1b.
* Click the peak with correct d spacing in the 1D spectrum viewer as shown in Fig. 1c.
* Close the Instrument View window as in Fig.1d.
* Repeat for each of the peaks listed in the script.

## 3.2 ROI Method

|  |  |
| --- | --- |
| a | b |
| c | d |

Figure 2 – Instrument Viewer in ROI mode

The Instrument View interface will open for each of the instances of run number in the list. The d-spacing limits will be set automatically based on (calculated peak d-spacing) ± (d tolerance + 0.1)

* To ease peak visibility, you can change the max counts on the colour map as shown in Fig 2a.
* If required, zoom into the region containing your peak as shown in Fig. 2b.
* Switch to the Draw tab (Fig. 2b) and select the ROI radio button (Fig 2c).
* Use the draw rectangle/ellipse tool to draw the region of interest (ROI) containing the peak as shown in Fig. 2c.
* Click Apply and Save, As Detector ROI to workspace and exit viewer as shown in Fig 2d.

This method will integrate each pixel with limits of expected d-spacing ± d-tolerance in this workspace to find the pixel with greatest value. This should return the pixel with the highest intensity at desired peak d-spacing. It will add this peak to the Peak table workspace.

# Section 4: Calculate UB methods

## ONE\_PEAK

This method calculates the UB matrix based on a single peak and a defined scattering plane. It makes use of the Mantid algorithm FindUBFromScatteringPlane.

* Takes the following inputs: lattice parameters, 2 vectors defining the scattering plane, and a Peaks workspace containing a peak in the scattering plane.
* If multiple peaks are supplied this algorithm takes the first entry in the Peak workspace.
* A warning will be raised if your chosen peak’s Miller indices are not within 5 deg of the plane.
* The up direction relative to the unit cell is unable to be determined so the output is dependent on the order vector\_1 and vector\_2 are entered, and can result in changing the sign of components above and below the scattering plane.
* This algorithm assumes the direction perpendicular to the measured peak is perfectly in the plane, so there is a loss of accuracy in determining the UB matrix when compared to other methods. The other methods that require more peaks will give a more accurate result (see below).

## TWO\_PEAKS

This method calculates the UB matrix using 2 peaks and does not refine any lattice parameters. It makes use of the Mantid algorithm CalculateUMatrix

* Takes the following inputs: lattice parameters, Peaks workspace containing a minimum of 2 peaks.
* Gives B from lattice parameters, and calculates the corresponding U matrix[[1]](#footnote-1)

## THREE\_PEAKS

This method calculates the UB matrix from 3 peaks, which does not require the use of the lattice constants. It makes use of the Mantid algorithm FindUBUsingIndexedPeaks

* This takes 2 inputs, a Peaks workspace containing at least 3 indexed peaks, and the tolerance on the calculated hkl values. This is the tolerance specified in Section 2.2.

## FIVEPLUS\_PEAKS

This method refines the UB matrix and lattice parameters, requiring the use of at least 5 peaks. It makes use of the Mantid algorithm Uses FindUBUsingLatticeParameters,

* Takes lattice parameters as inputs and a PeaksWorkspace containing at least 5 peaks.

# Section 5: Reorientation

## 5.1 Psi Rotation

* Rotation about the vertical direction is optimised to map peak to u vector
* This rotation is then applied to the UB matrix
* The angle of rotation is also printed

## 5.2 Phi Rotation

* Angle of Rotation about Axis1 or the X axis (in the instrument frame) if second rotation axis is not specified - is optimised to map provided peak to beam direction.
* This optimisation occurs after the Psi optimisation and is not applied to the UB matrix.
* The Angle is outputted to the user, positive is anticlockwise rotation about the axis, negative is clockwise. This indicates how far out of the scattering plane the specified peak is in degrees.
* For positive x axis, a positive angle indicates that offset below the plane, negative is above the plane.

# Section 6 Verification Methods

## 6.1 Peak Prediction & Use

* Peaks are predicted from the UB set on the Single Crystal workspace first in the list
* The prior entered reflection condition/ crystal structure (details in Section 1.4) is used to predict the Qs of peaks in a given d spacing range
* A screenshot of a computer

  AI-generated content may be incorrect.The resulting workspace can be dragged and dropped onto instrument viewer to visualise the peaks

Figure 3 – Instrument viewer with Predict Peaks Overlay

# Appendix 1: Text File Output

The script generates an output file named DG\_Alignment\_Output\_{date\_and\_time}. The contents of the file depend on Reorient flag value:

* When Reorient = False:  
  The file will include the following details:
  + The UB method used for the calculation
  + The UB matrix
  + The **u** and **v** vectors
* When Reorient = True:  
  In addition to the information listed above, the file will contain an extra section with:
  + The rotation required to align the peak
  + The updated UB matrix after rotation
  + The modified **u** and **v** vectors following the alignment process

An example is shown below:

A screenshot of a computer

AI-generated content may be incorrect.

# Appendix 2: Class Definitions File

This file defines custom classes for instrument specifications and utilizes Enum to delineate the various methods selected within the script.

Instrument Class

The Instrument class requires two arguments:

1. Instrument Name: A string representing the name of the instrument.
2. Axis Dictionary: A dictionary where the keys are labeled Axis{n} (e.g., Axis1, Axis2) and the corresponding values are strings specifying the axis details in the format: "axisname,x,y,z,±1".

The class contains predefined objects for specific instruments such asMAPS, MERLIN,and LET.

Enum Class Definitions

The script includes several Enum classes to define method options. The available options within each class are as follows:

Reflection Conditions (reflection\_condition):

* PRIMITIVE: "Primitive"
* BODY\_CENTERED: "Body Centered"
* C\_FACE\_CENTERED: "C-face centered"
* B\_FACE\_CENTERED: "B-face centered"
* A\_FACE\_CENTERED: "A-face centered"
* ALL\_FACE\_CENTERED: "All-face centered"
* RHOMBO\_CENTERED\_REV: "Rhombohedrally centered reverse"
* HEX\_CENTERED\_REV: "Hexagonally centered, reverse"

UB Calculation Methods (UB\_methods):

* ONE\_PEAK: "One peak"
* TWO\_PEAKS: "Two peaks"
* THREE\_PEAKS: "Three peaks"
* FIVEPLUS\_PEAKS: "Five or more peaks"

Peak Picking Methods (Peak\_picking\_methods):

* MANUAL: "Manual"
* ROI: "Region of Interest (ROI)"

Beam Modes (beam\_modes Enum):

* WHITE\_BEAM: "White beam"
* MONOCHROMATIC: "Monochromatic"

# Appendix 3: Adding Additional Instruments

The class definition file referred in Appendix 2 contains an Instrument class, this class can be called to construct a new instrument. Construction must be in the following format:

E.g

axes = {  
 "Axis0" : "Rot,0,1,0,1"

“Axis1”: “Phi,0,0,1”  
}  
MAPS = Instrument("MAPS",axes)

axes\_name = {

“Axis0” = “Axis\_name,x,y,z,±1”

…

}

Instrument\_Name = Instrument(“Instrument\_name”, axes\_name)

# Appendix 4: List of Space Groups

List of allowed space group symbols ordered by space group number

|  |  |
| --- | --- |
| Number | Space Group Symbols |
| 1 | P 1 |
| 2 | P -1 |
| 3 | P 1 1 2, P 1 2 1 |
| 4 | P 1 1 21, P 1 21 1 |
| 5 | A 1 1 2, A 1 2 1, B 1 1 2, C 1 2 1, I 1 1 2, I 1 2 1 |
| 6 | P 1 1 m, P 1 m 1 |
| 7 | P 1 1 a, P 1 1 b, P 1 1 n, P 1 a 1, P 1 c 1, P 1 n 1 |
| 8 | A 1 1 m, A 1 m 1, B 1 1 m, C 1 m 1, I 1 1 m, I 1 m 1 |
| 9 | A 1 1 a, A 1 n 1, B 1 1 n, C 1 c 1, I 1 1 b, I 1 a 1 |
| 10 | P 1 1 2/m, P 1 2/m 1 |
| 11 | P 1 1 21/m, P 1 21/m 1 |
| 12 | A 1 1 2/m, A 1 2/m 1, B 1 1 2/m, C 1 2/m 1, I 1 1 2/m, I 1 2/m 1 |
| 13 | P 1 1 2/a, P 1 1 2/b, P 1 1 2/n, P 1 2/a 1, P 1 2/c 1, P 1 2/n 1 |
| 14 | P 1 1 21/a, P 1 1 21/b, P 1 1 21/n, P 1 21/a 1, P 1 21/c 1, P 1 21/n 1 |
| 15 | A 1 1 2/a, A 1 2/n 1, B 1 1 2/n, C 1 2/c 1, I 1 1 2/b, I 1 2/a 1 |
| 16 | P 2 2 2 |
| 17 | P 2 2 21, P 2 21 2, P 21 2 2 |
| 18 | P 2 21 21, P 21 2 21, P 21 21 2 |
| 19 | P 21 21 21 |
| 20 | A 21 2 2, B 2 21 2, C 2 2 21 |
| 21 | A 2 2 2, B 2 2 2, C 2 2 2 |
| 22 | F 2 2 2 |
| 23 | I 2 2 2 |
| 24 | I 21 21 21 |
| 25 | P 2 m m, P m 2 m, P m m 2 |
| 26 | P 21 a m, P 21 m a, P b 21 m, P c m 21, P m 21 b, P m c 21 |
| 27 | P 2 a a, P b 2 b, P c c 2 |
| 28 | P 2 c m, P 2 m b, P b m 2, P c 2 m, P m 2 a, P m a 2 |
| 29 | P 21 a b, P 21 c a, P b 21 a, P b c 21, P c 21 b, P c a 21 |
| 30 | P 2 a n, P 2 n a, P b 2 n, P c n 2, P n 2 b, P n c 2 |
| 31 | P 21 m n, P 21 n m, P m 21 n, P m n 21, P n 21 m, P n m 21 |
| 32 | P 2 c b, P b a 2, P c 2 a |
| 33 | P 21 c n, P 21 n b, P b n 21, P c 21 n, P n 21 a, P n a 21 |
| 34 | P 2 n n, P n 2 n, P n n 2 |
| 35 | A 2 m m, B m 2 m, C m m 2 |
| 36 | A 21 a m, A 21 m a, B b 21 m, B m 21 b, C c m 21, C m c 21 |
| 37 | A 2 a a, B b 2 b, C c c 2 |
| 38 | A m 2 m, A m m 2, B 2 m m, B m m 2, C 2 m m, C m 2 m |
| 39 | A e 2 m, A e m 2, B 2 e m, B m e 2, C 2 m e, C m 2 e |
| 40 | A m 2 a, A m a 2, B 2 m b, B b m 2, C 2 c m, C c 2 m |
| 41 | A e 2 a, A e a 2, B 2 e b, B b e 2, C 2 c e, C c 2 e |
| 42 | F 2 m m, F m 2 m, F m m 2 |
| 43 | F 2 d d, F d 2 d, F d d 2 |
| 44 | I 2 m m, I m 2 m, I m m 2 |
| 45 | I 2 c b, I b a 2, I c 2 a |
| 46 | I 2 c m, I 2 m b, I b m 2, I c 2 m, I m 2 a, I m a 2 |
| 47 | P m m m |
| 48 | P n n n, P n n n :2 |
| 49 | P b m b, P c c m, P m a a |
| 50 | P b a n, P b a n :2, P c n a, P c n a :2, P n c b, P n c b :2 |
| 51 | P b m m, P c m m, P m a m, P m c m, P m m a, P m m b |
| 52 | P b n n, P c n n, P n a n, P n c n, P n n a, P n n b |
| 53 | P b m n, P c n m, P m a n, P m n a, P n c m, P n m b |
| 54 | P b a a, P b a b, P b c b, P c a a, P c c a, P c c b |
| 55 | P b a m, P c m a, P m c b |
| 56 | P b n b, P c c n, P n a a |
| 57 | P b c m, P b m a, P c a m, P c m b, P m a b, P m c a |
| 58 | P m n n, P n m n, P n n m |
| 59 | P m m n, P m m n :2, P m n m, P m n m :2, P n m m, P n m m :2 |
| 60 | P b c n, P b n a, P c a n, P c n b, P n a b, P n c a |
| 61 | P b c a, P c a b |
| 62 | P b n m, P c m n, P m c n, P m n b, P n a m, P n m b |
| 63 | P m c b, P m c a, P m a n |
| 64 | P 43 2 2, P 42 3 2 |
| 65 | P 432, P 422 |
| 66 | F 432, F 422 |
| 67 | I 432, I 422 |
| 68 | P 42 3 2 |
| 69 | P 43 3 2 |
| 70 | P 4321 |
| 71 | P 42 3 |
| 72 | P 43 2 |
| 73 | F 43 2 |
| 74 | F 42 3 |
| 75 | F 41 3 2 |
| 76 | F 41 3 2 |
| 77 | I 41 3 2 |
| 78 | I 41 3 2 |
| 79 | P -4 3 m |
| 80 | F -4 3 m |
| 81 | I -4 3 m |
| 82 | P -4 3 n |
| 83 | F -4 3 c |
| 84 | I -4 3 d |
| 85 | P m -3 m |
| 86 | P n -3 n, P n -3 n :2 |
| 87 | P m -3 n |
| 88 | P n -3 m, P n -3 m :2 |
| 89 | F m -3 m |
| 90 | F m -3 c |
| 91 | F d -3 m, F d -3 m :2 |
| 92 | F d -3 c, F d -3 c :2 |
| 93 | I m -3 m |
| 94 | I m -3 c |
| 95 | I a -3 d |
| 96 | I 4 |
| 97 | I 41 |
| 98 | P 4 |
| 99 | P 41 |
| 100 | P 42 |
| 101 | P 43 |
| 102 | I 4 |
| 103 | I 41 |
| 104 | P 4 |
| 105 | P 41 |
| 106 | P 42 |
| 107 | P 43 |
| 108 | P 4 |
| 109 | P 41 |
| 110 | P 42 |
| 111 | P 43 |
| 112 | P -4 |
| 113 | P 41 |
| 114 | P 42 |
| 115 | P 43 |
| 116 | P 4 |
| 117 | P 41 |
| 118 | P 42 |
| 119 | P 43 |
| 120 | P 4 |
| 121 | I 41 |
| 122 | I 42 |
| 123 | P 42 |
| 124 | P 43 |
| 125 | P 4 |
| 126 | P 41 |
| 127 | P 42 |
| 128 | P 43 |
| 129 | P 4 |
| 130 | I a -3 d |
| 131 | P m -3 m |
| 132 | P -4 3 m |
| 133 | P -4 3 n |
| 134 | I m -3 c |
| 135 | I -4 3 c |
| 136 | F m -3 c |
| 137 | P n -3 m |
| 138 | F -4 3 c |
| 139 | I -4 3 m |
| 140 | I m -3 m |
| 141 | F d -3 m |
| 142 | I -4 3 n |
| 143 | F -4 3 m |
| 144 | I -4 3 c |
| 145 | I m -3 m |
| 146 | I 4 |
| 147 | I 41 |
| 148 | P 4 |
| 149 | P 41 |
| 150 | P 42 |
| 151 | P 43 |
| 152 | P -4 |
| 153 | P 41 |
| 154 | P 42 |
| 155 | P 43 |
| 156 | P 4 |
| 157 | I 41 |
| 158 | I 42 |
| 159 | P 42 |
| 160 | P 43 |
| 161 | P 4 |
| 162 | I 41 |
| 163 | I 42 |
| 164 | P 42 |
| 165 | P 43 |
| 166 | P 4 |
| 167 | I 41 |
| 168 | I 42 |
| 169 | P 42 |
| 170 | P 43 |
| 171 | P 4 |
| 172 | I a -3 d |
| 173 | P m -3 m |
| 174 | P -4 3 m |
| 175 | P -4 3 n |
| 176 | I m -3 c |
| 177 | I -4 3 c |
| 178 | F m -3 c |
| 179 | P n -3 m |
| 180 | F -4 3 c |
| 181 | I -4 3 m |
| 182 | I m -3 m |
| 183 | F d -3 m |
| 184 | I -4 3 n |
| 185 | F -4 3 m |
| 186 | I -4 3 c |
| 187 | I m -3 m |
| 188 | I 4 |
| 189 | I 41 |
| 190 | P 4 |
| 191 | P 41 |
| 192 | P 42 |
| 193 | P 43 |
| 194 | P -4 |
| 195 | P 41 |
| 196 | P 42 |
| 197 | P 43 |
| 198 | P 4 |
| 199 | I 41 |
| 200 | I 42 |
| 201 | P 42 |
| 202 | P 43 |
| 203 | P 4 |
| 204 | I 41 |
| 205 | I 42 |
| 206 | P 42 |
| 207 | P 43 |
| 208 | P 4 |
| 209 | I 41 |
| 210 | I 42 |
| 211 | P 42 |
| 212 | P 43 |
| 213 | P 4 |
| 214 | I 41l |
| 215 | I 42 |
| 216 | P 42 |
| 217 | P 43 |
| 218 | P 4 |
| 219 | I 41 |
| 220 | I 42 |
| 221 | P 42 |
| 222 | P 43 |
| 223 | P 4 |
| 224 | I 41 |
| 225 | I 42 |
| 226 | P 42 |
| 227 | P 43 |
| 228 | P 4 |
| 229 | I 41 |
| 230 | I 42 |

1. U matrix is found by minimising square difference between Qlab and Qlab predicted [↑](#footnote-ref-1)