Experiences with Twinning

Jim Britten (McMaster)

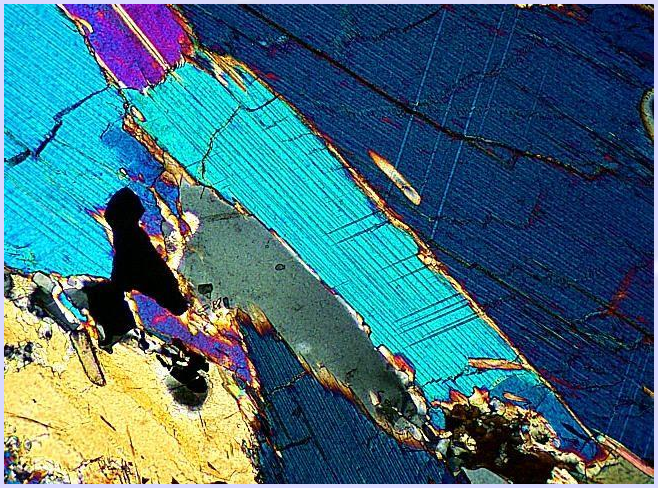
With a lot of input from Regine Herbst-Irmer (Gottingen) and Ton Spek (Utrecht)

Outline

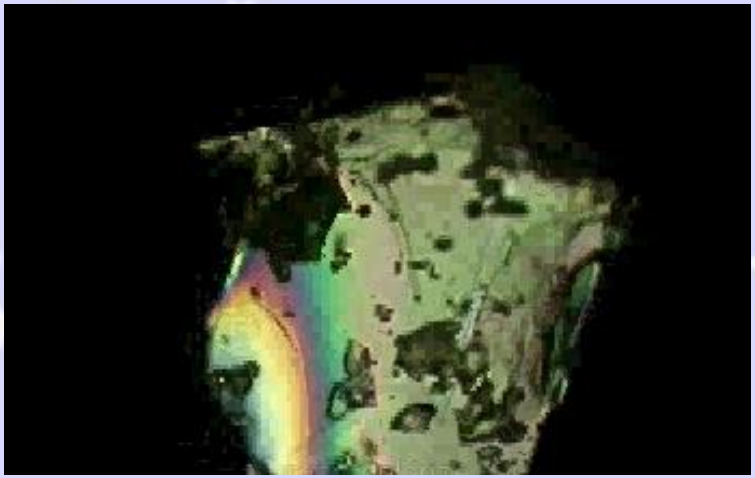
- Twinned crystal growth
- Merohedral twinning
- Non-merohedral twinning
- Pseudo-merohedral twinning
- Twinning that isn’t twinning

“Twins are regular aggregates consisting of individual crystals of the same species joined together in some definite mutual orientation.”

from: "Fundamentals of Crystallography", edited by C. Giacovazzo, Union of Crystallography, Oxford University Press 2nd Edn. 2002.



Cross-polarized microscope image of a twinned crystal. (https://i.pinimg.com/originals/49/9c/38/499c3896dd4e84bdad20dbe8b4f9e4a2.jpg)



Cross-polarized microscope image of a single crystal with powder grains on the surface.

Merohedral Twinning

The twin operator is a symmetry operator of the crystal system but not of the point group of the crystal. The result is a 100% overlap of reflections from each component.

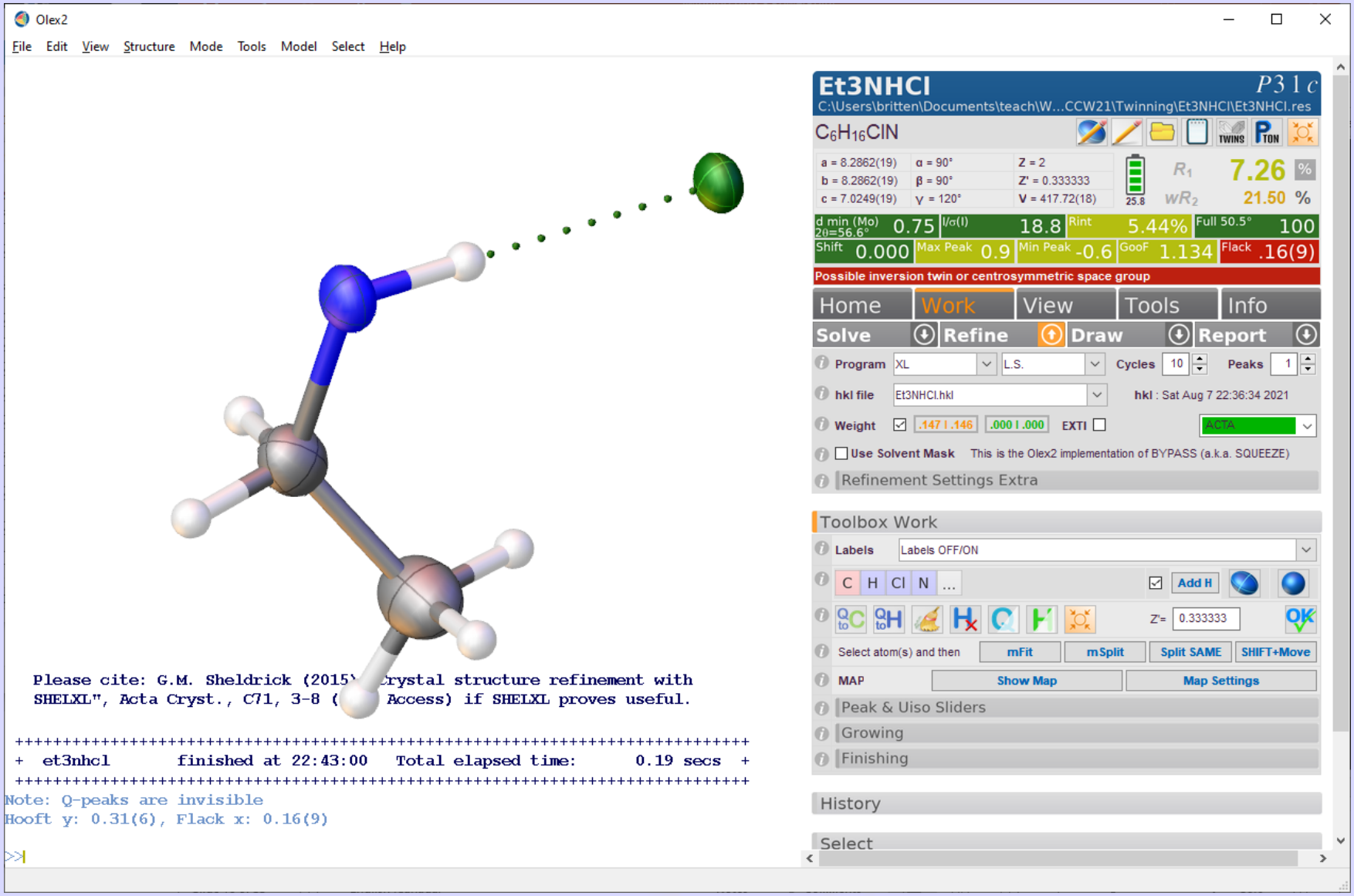
This includes racemic twinning for a non centrosymmetric structure (inverted packing). i.e. The space group of the structure does not have a center of symmetry, but the twin component has the inverted structure of the main crystal.

Merohedral twinning can also be due to an operator not part of the Laue group of the crystal. This can only occur for lower symmetry trigonal, tetragonal, hexagonal and cubic space groups. For example, a twinned crystal growing with P4/m symmetry may give a diffraction pattern that appears to have P4/mmm symmetry.

Warning Signs for Merohedral Twinning

- Metric symmetry higher than Laue symmetry
- R_{int} for the higher symmetry Laue group only slightly higher than for the lower symmetry one
- Different R_{int} values for the higher symmetry Laue group for different crystals of the same compound
- Mean value for $|E^2 - 1| << 0.736$
- Apparent trigonal or hexagonal space group
- Systematic absences not consistent with any known space group
- No structure solution
- Patterson function physically impossible (for heavy atom structures)
- High R-Values

Regine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P31c
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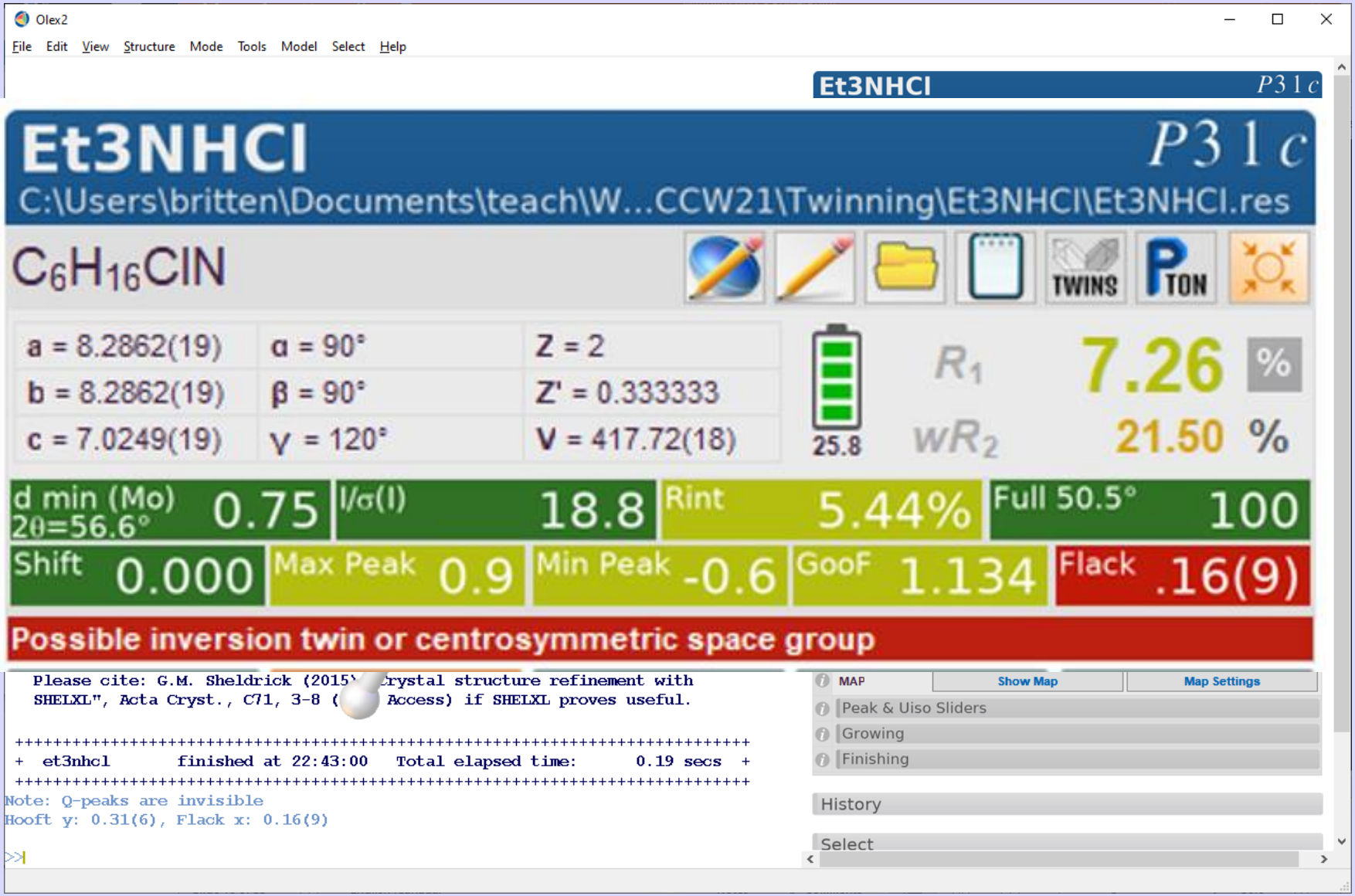
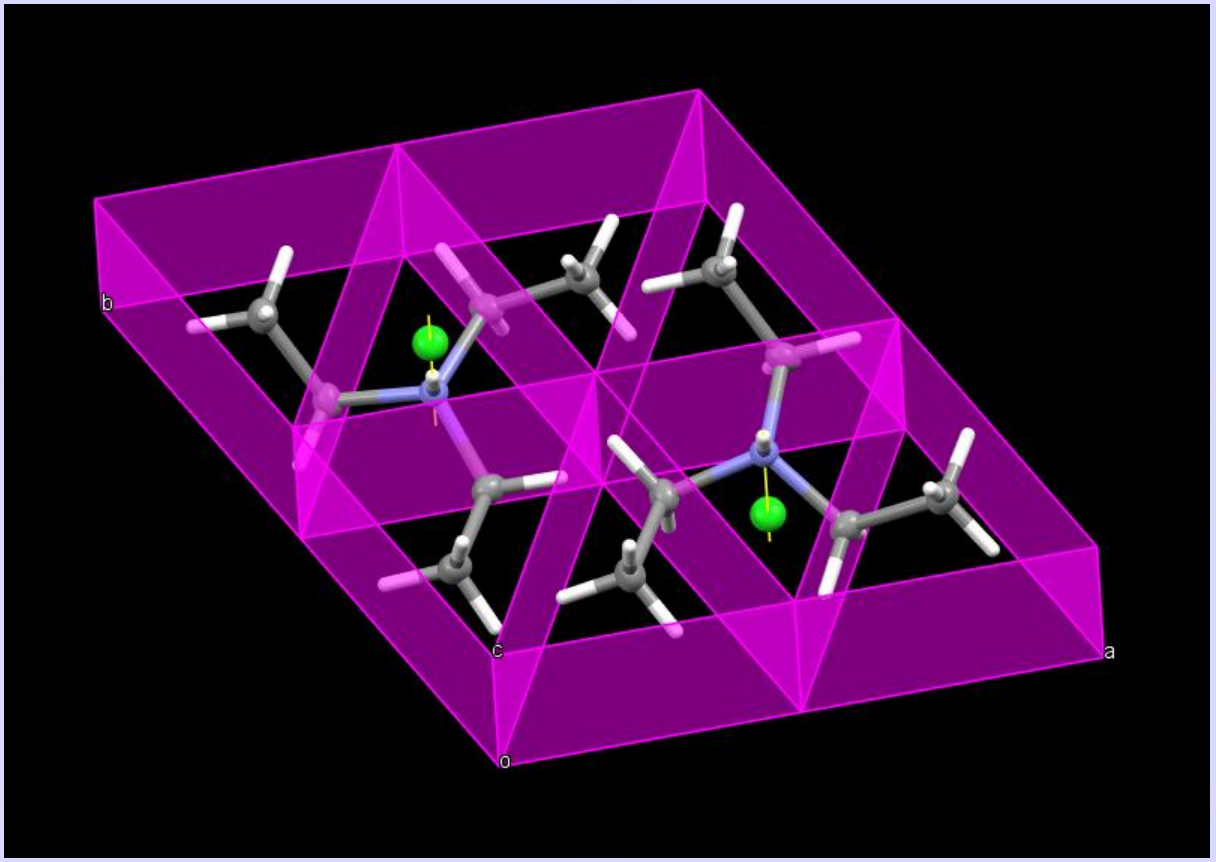
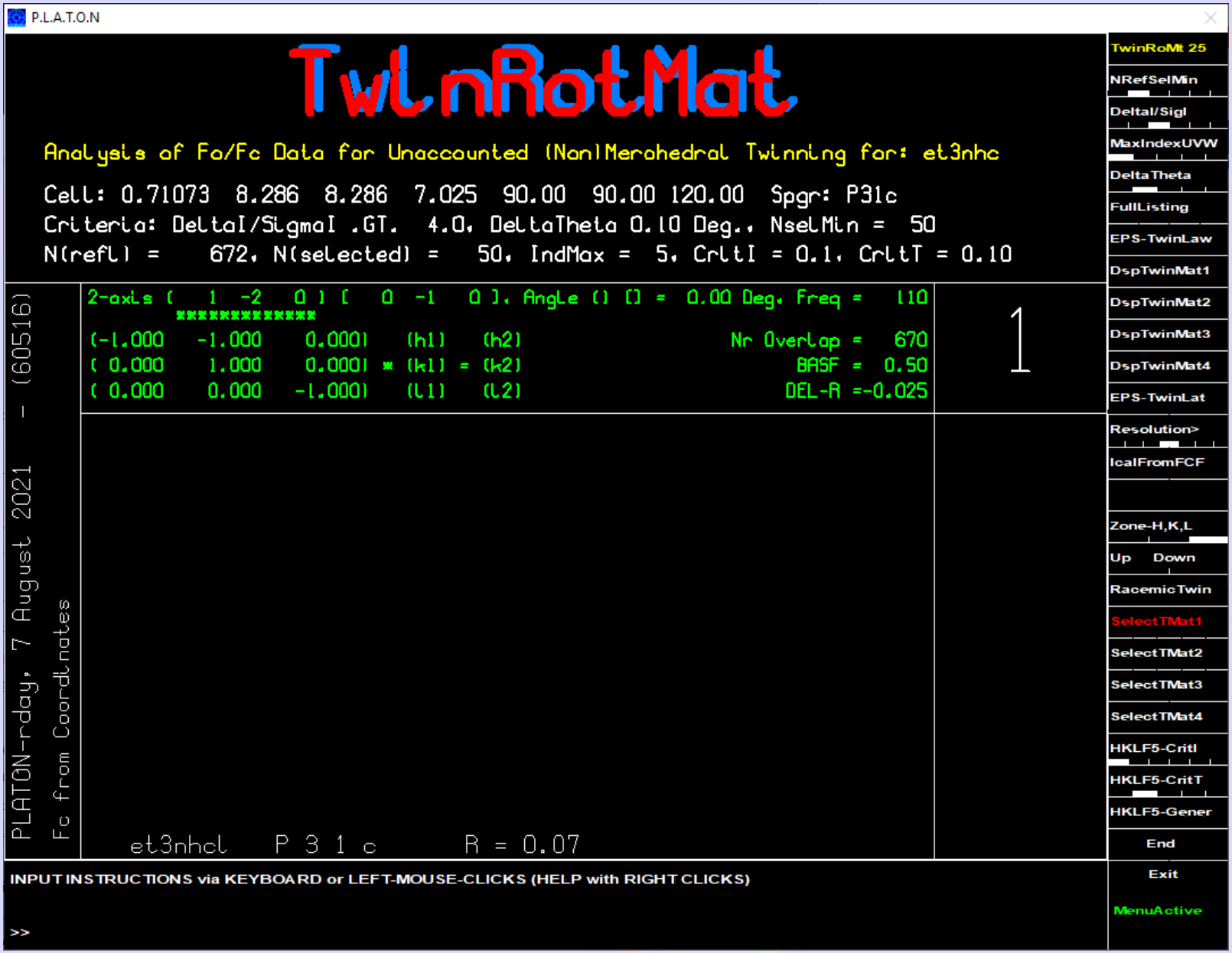
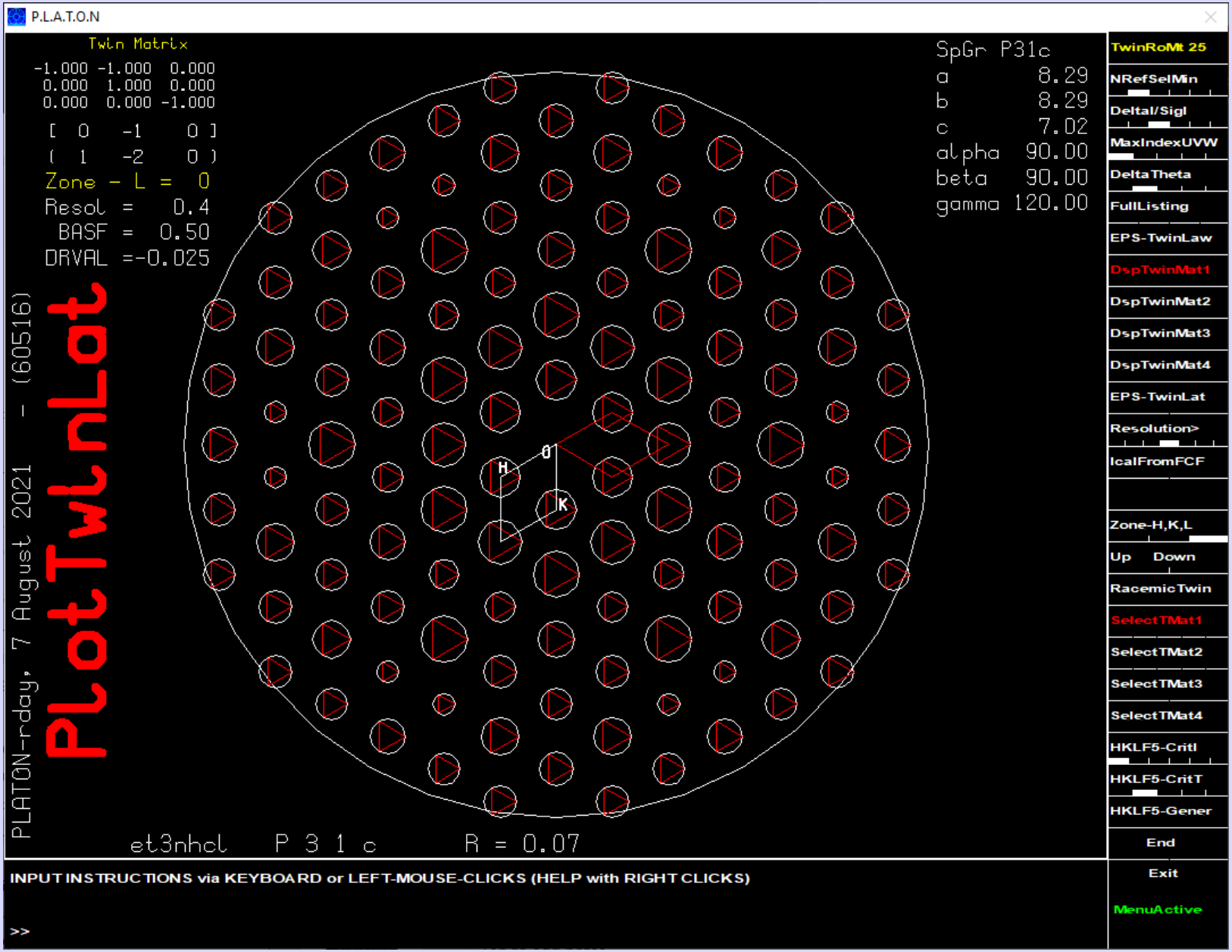
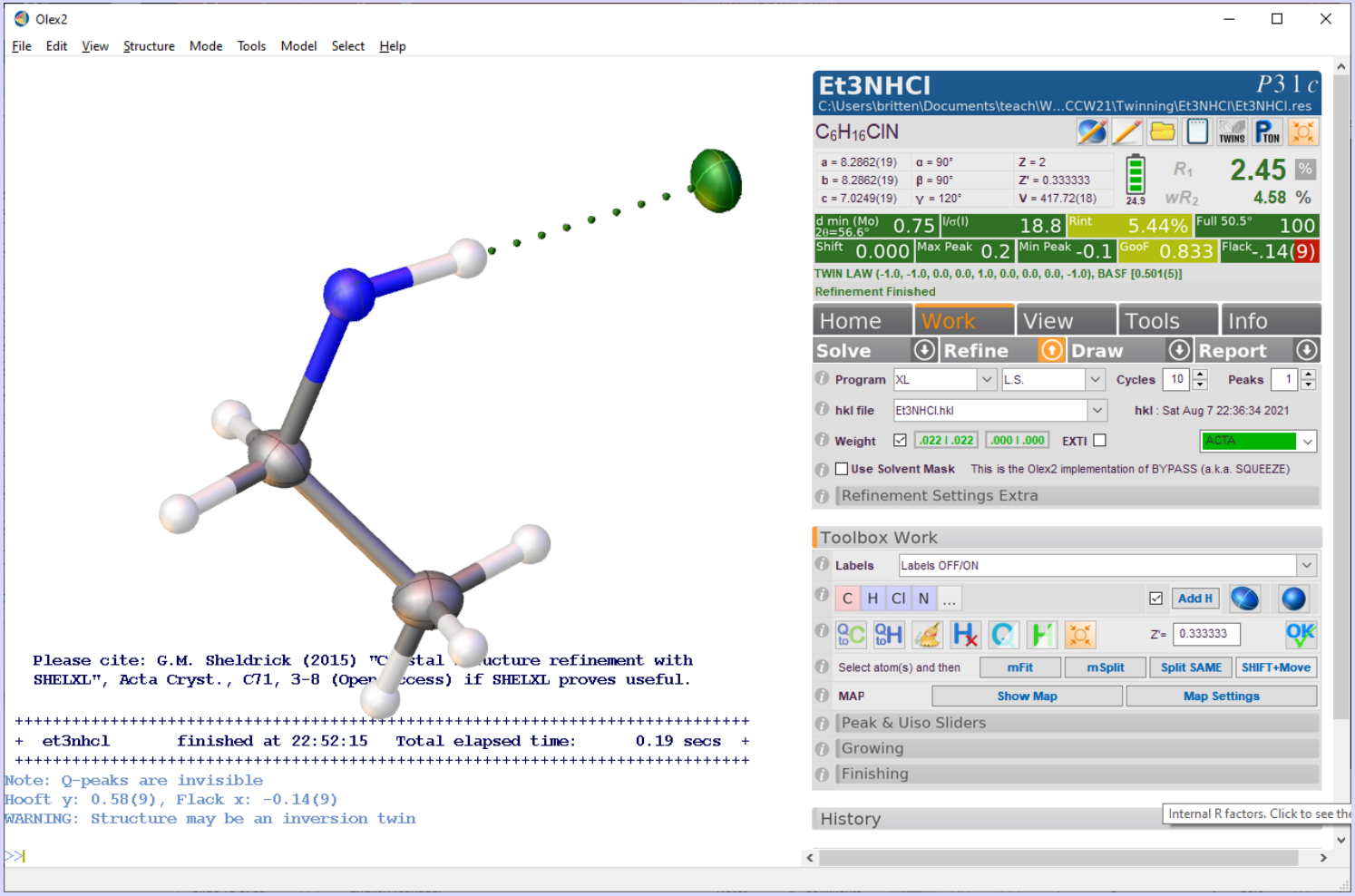
C6H16ClN
a = 8.2862(19) α = 90° Z = 2
b = 8.2862(19) β = 90° Z' = 0.333333
c = 7.0249(19) γ = 120° V = 417.72(18)
25.8
R1 7.26 %
wR2 21.50 %
d min (Mo) 2θ=56.6° 0.75
I/σ(I) 18.8
Rint 5.44%
Full 50.5° 100
Shift 0.000
Max Peak 0.9
Min Peak -0.6
GooF 1.134
Flack .16(9)
Possible inversion twin or centrosymmetric space group
Home Work View Tools Info
Solve Refine Draw Report
Program XL L.S. Cycles 10 Peaks 1
hkl file Et3NHCl.hkl hkl : Sat Aug 7 22:36:34 2021
Weight .147 1.146 .000 1.000 EXTI ACTA
Use Solvent Mask This is the Olex2 implementation of BYPASS (a.k.a. SQUEEZE)
Refinement Settings Extra
Toolbox Work
Labels Labels OFF/ON
C H Cl N ... Add H
Z'= 0.333333
Select atom(s) and then mFit mSplit Split SAME SHIFT+Move
MAP Show Map Map Settings
Peak & Uiso Sliders
Growing
Finishing
History
Select
Please cite: G.M. Sheldrick (2015) Crystal structure refinement with SHELXL", Acta Cryst., C71, 3-8 (Access) if SHELXL proves useful.
+ et3nhcl finished at 22:43:00 Total elapsed time: 0.19 secs +
Note: Q-peaks are invisible
Hooft y: 0.31(6), Flack x: 0.16(9)
>>

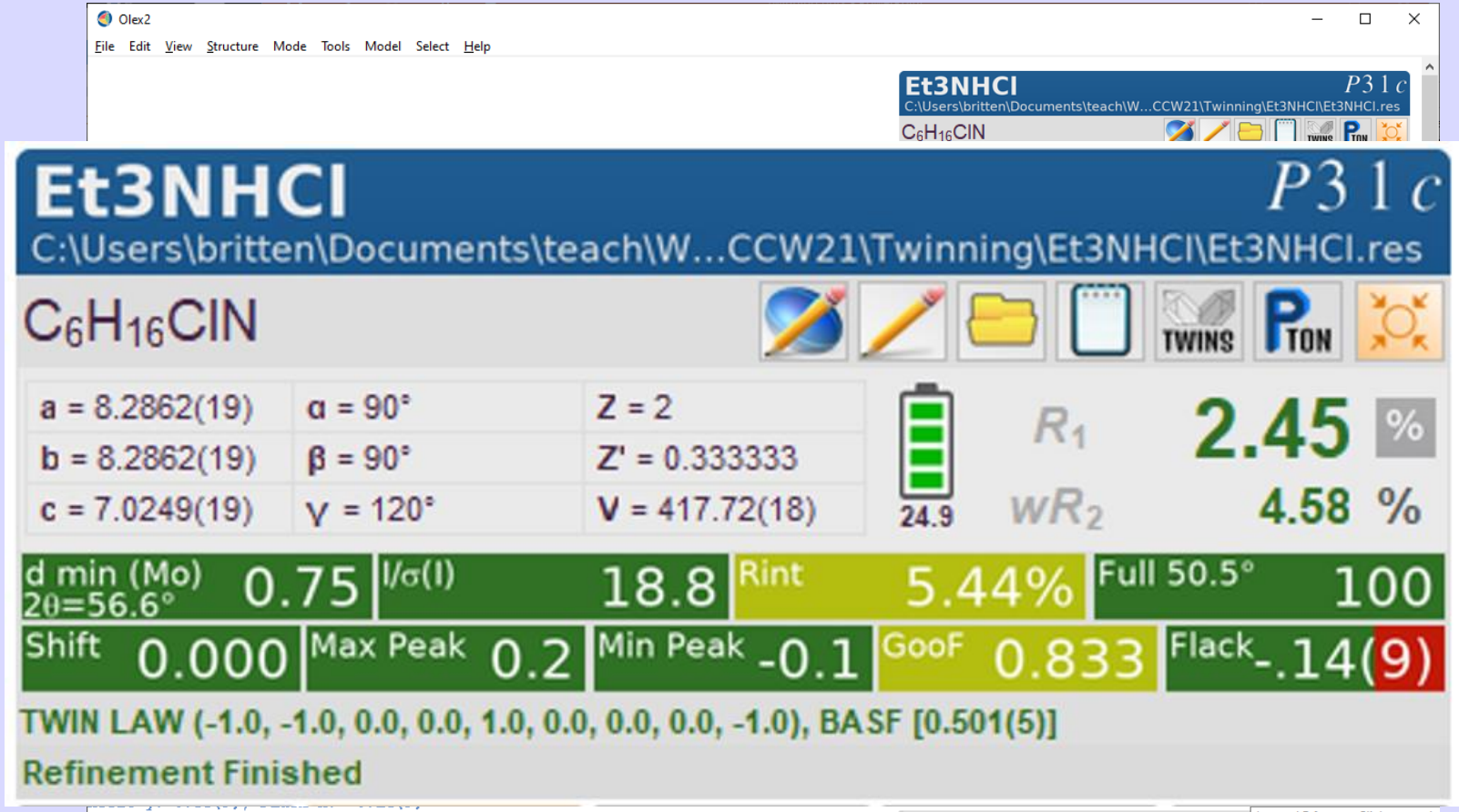

Olex2
File Edit View Structure Mode Tools Model Select Help
Et3NHCl P31c
Et3NHCl P31c
C:\Users\britten\Documents\teach\W...CCW21\Twinning\Et3NHCl\Et3NHCl.res
C6H16ClN
TWINS
PTON
a = 8.2862(19) α = 90° Z = 2
b = 8.2862(19) β = 90° Z' = 0.333333
c = 7.0249(19) γ = 120° V = 417.72(18)
25.8
R1 7.26 %
wR2 21.50 %
d min (Mo) 2θ=56.6° 0.75
I/σ(I) 18.8
Rint 5.44%
Full 50.5° 100
Shift 0.000
Max Peak 0.9
Min Peak -0.6
GooF 1.134
Flack .16(9)
Possible inversion twin or centrosymmetric space group
Please cite: G.M. Sheldrick (2015) Crystal structure refinement with SHELXL", Acta Cryst., C71, 3-8 (Access) if SHELXL proves useful.
et3nhcl finished at 22:43:00 Total elapsed time: 0.19 secs
Note: Q-peaks are invisible
Hooft y: 0.31(6), Flack x: 0.16(9)
>>
MAP
Show Map
Map Settings
Peak & Uiso Sliders
Growing
Finishing
History
Select


b
c
a
o


P.L.A.T.O.N
TwlnRotMat
Analysis of Fo/Fc Data for Unaccounted (Non)Merohedral Twinning for: et3nhc
Cell: 0.71073 8.286 8.286 7.025 90.00 90.00 120.00 Spgr: P31c
Criteria: DeltaI/SigmaI .GT. 4.0, DeltaTheta 0.10 Deg., NselMin = 50
N(refl) = 672, N(selected) = 50, IndMax = 5, CrltI = 0.1, CrltT = 0.10
2-axis (1 -2 0) [0 -1 0], Angle () [] = 0.00 Deg. Freq = 110
(-1.000 -1.000 0.000) (h1) (h2) Nr Overlap = 670
(0.000 1.000 0.000) * (k1) = (k2) BASF = 0.50
(0.000 0.000 -1.000) (l1) (l2) DEL-R =-0.025
1
PLATON-rday, 7 August 2021 - (60516)
Fc from Coordinates
et3nhcl P 3 1 c R = 0.07
INPUT INSTRUCTIONS via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
TwinRoMt 25
NRefSelMin
DeltaI/SigI
MaxIndexUVW
DeltaTheta
FullListing
EPS-TwinLaw
DspTwinMat1
DspTwinMat2
DspTwinMat3
DspTwinMat4
EPS-TwinLat
Resolution>
IcalFromFCF
Zone-H,K,L
Up Down
RacemicTwin
SelectTMat1
SelectTMat2
SelectTMat3
SelectTMat4
HKLF5-CritI
HKLF5-CritT
HKLF5-Gener
End
Exit
MenuActive


P.L.A.T.O.N
Twin Matrix
-1.000 -1.000 0.000
0.000 1.000 0.000
0.000 0.000 -1.000
[0 -1 0]
(1 -2 0)
Zone - L = 0
Resol = 0.4
BASF = 0.50
DRVAL =-0.025
SpGr P31c
a 8.29
b 8.29
c 7.02
alpha 90.00
beta 90.00
gamma 120.00
PLATON-rday, 7 August 2021 - (60516)
PlotTwLnLat
H
O
K
et3nhcl P 3 1 c R = 0.07
TwinRoMt 25
NRefSelMin
Deltal/Sigl
MaxIndexUVW
DeltaTheta
FullListing
EPS-TwinLaw
DspTwinMat1
DspTwinMat2
DspTwinMat3
DspTwinMat4
EPS-TwinLat
Resolution>
IcalFromFCF
Zone-H,K,L
Up Down
RacemicTwin
SelectTMat1
SelectTMat2
SelectTMat3
SelectTMat4
HKLF5-CritI
HKLF5-CritT
HKLF5-Gener
End
Exit
MenuActive
INPUT INSTRUCTIONS via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>


Olex2
File Edit View Structure Mode Tools Model Select Help
Et3NHCl
P31c
C:\Users\britten\Documents\teach\W...CCW21\Twinning\Et3NHCl\Et3NHCl.res
C6H16ClN
a = 8.2862(19) α = 90° Z = 2
b = 8.2862(19) β = 90° Z' = 0.333333
c = 7.0249(19) γ = 120° V = 417.72(18)
R1 2.45 %
wR2 4.58 %
d min (Mo) 2θ=56.6° 0.75 I/σ(I) 18.8 Rint 5.44% Full 50.5° 100
Shift 0.000 Max Peak 0.2 Min Peak -0.1 GooF 0.833 Flack -.14(9)
TWIN LAW (-1.0, -1.0, 0.0, 0.0, 1.0, 0.0, 0.0, 0.0, -1.0), BASF [0.501(5)]
Refinement Finished
Home Work View Tools Info
Solve Refine Draw Report
Program XL L.S. Cycles 10 Peaks 1
hkl file Et3NHCl.hkl hkl : Sat Aug 7 22:36:34 2021
Weight .022 I .022 .000 I .000 EXTI
Use Solvent Mask This is the Olex2 implementation of BYPASS (a.k.a. SQUEEZE)
Refinement Settings Extra
Toolbox Work
Labels Labels OFF/ON
C H Cl N ...
Add H
Z'= 0.333333
Select atom(s) and then mFit mSplit Split SAME SHIFT+Move
MAP Show Map Map Settings
Peak & Uiso Sliders
Growing
Finishing
History
Internal R factors. Click to see the
Please cite: G.M. Sheldrick (2015) "Crystal structure refinement with SHELXL", Acta Cryst., C71, 3-8 (Open Access) if SHELXL proves useful.
+ et3nhcl finished at 22:52:15 Total elapsed time: 0.19 secs +
Note: Q-peaks are invisible
Hooft y: 0.58(9), Flack x: -0.14(9)
WARNING: Structure may be an inversion twin
>>


Olex2
File Edit View Structure Mode Tools Model Select Help
Et3NHCl P31c
C:\Users\britten\Documents\teach\W...CCW21\Twinning\Et3NHCl\Et3NHCl.res
C6H16ClN
Et3NHCl P31c
C:\Users\britten\Documents\teach\W...CCW21\Twinning\Et3NHCl\Et3NHCl.res
C6H16ClN
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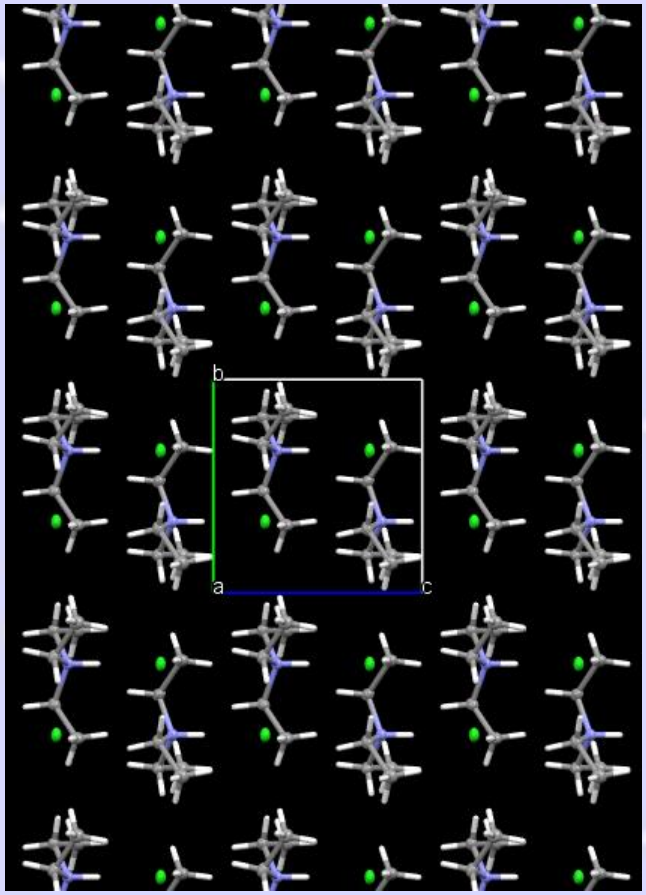
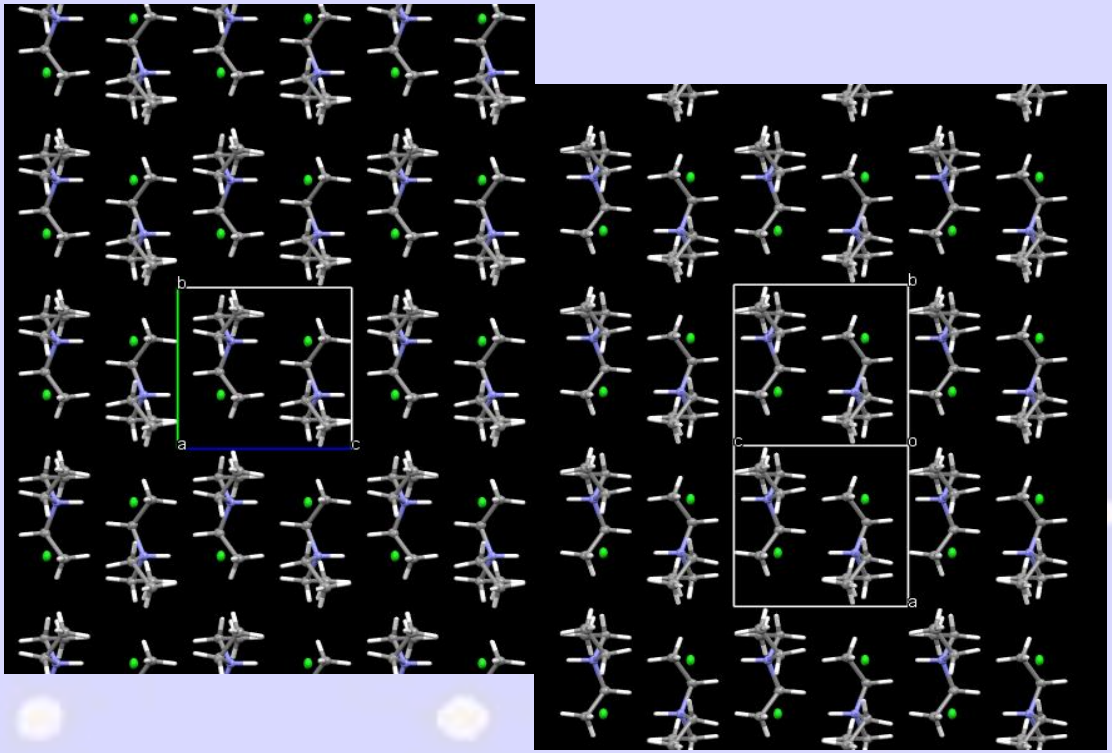
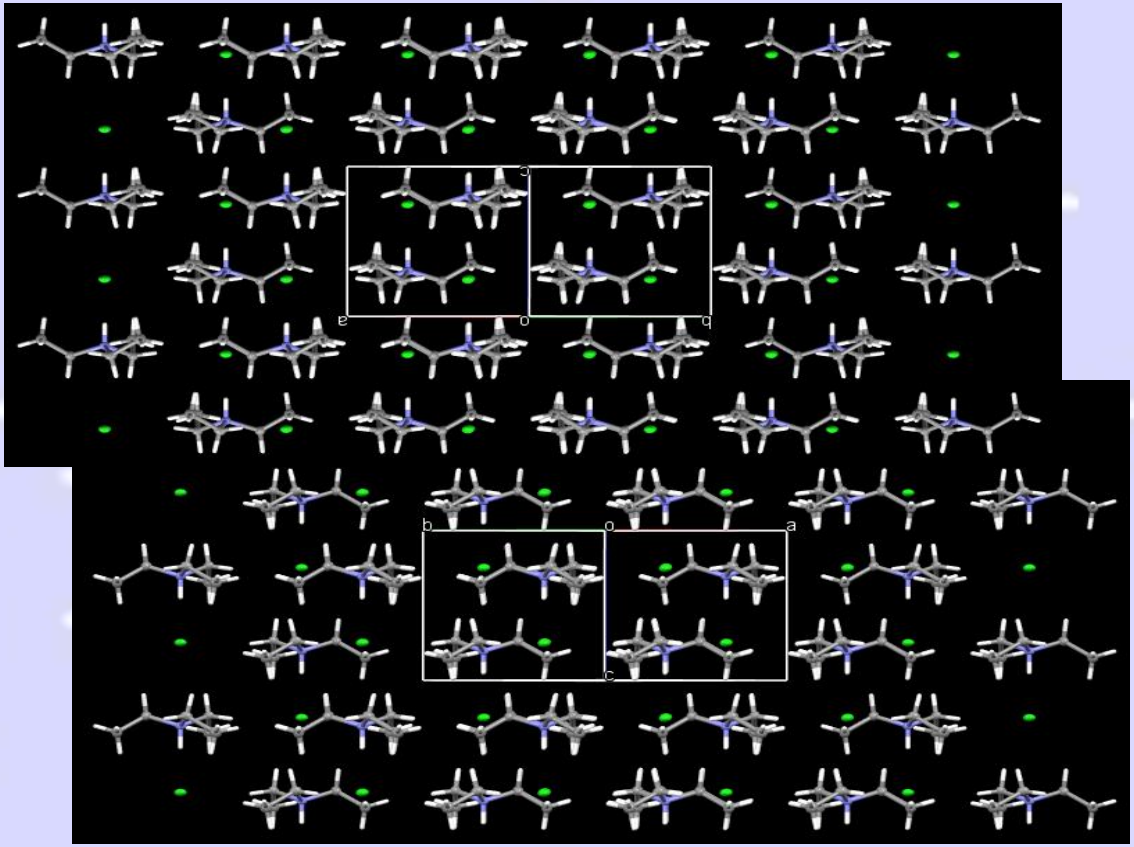
wR2 4.58 %
d min (Mo) 2θ=56.6° 0.75
I/σ(I) 18.8
Rint 5.44%
Full 50.5° 100
Shift 0.000
Max Peak 0.2
Min Peak -0.1
GooF 0.833
Flack -.14(9)
TWIN LAW (-1.0, -1.0, 0.0, 0.0, 1.0, 0.0, 0.0, 0.0, -1.0), BASF [0.501(5)]
Refinement Finished
WARNING: Structure may be an inversion twin
History
Internal R factors. Click to see the
>>

Crystal structure of [Et3N]Cl as displayed in CCDC's Mercury

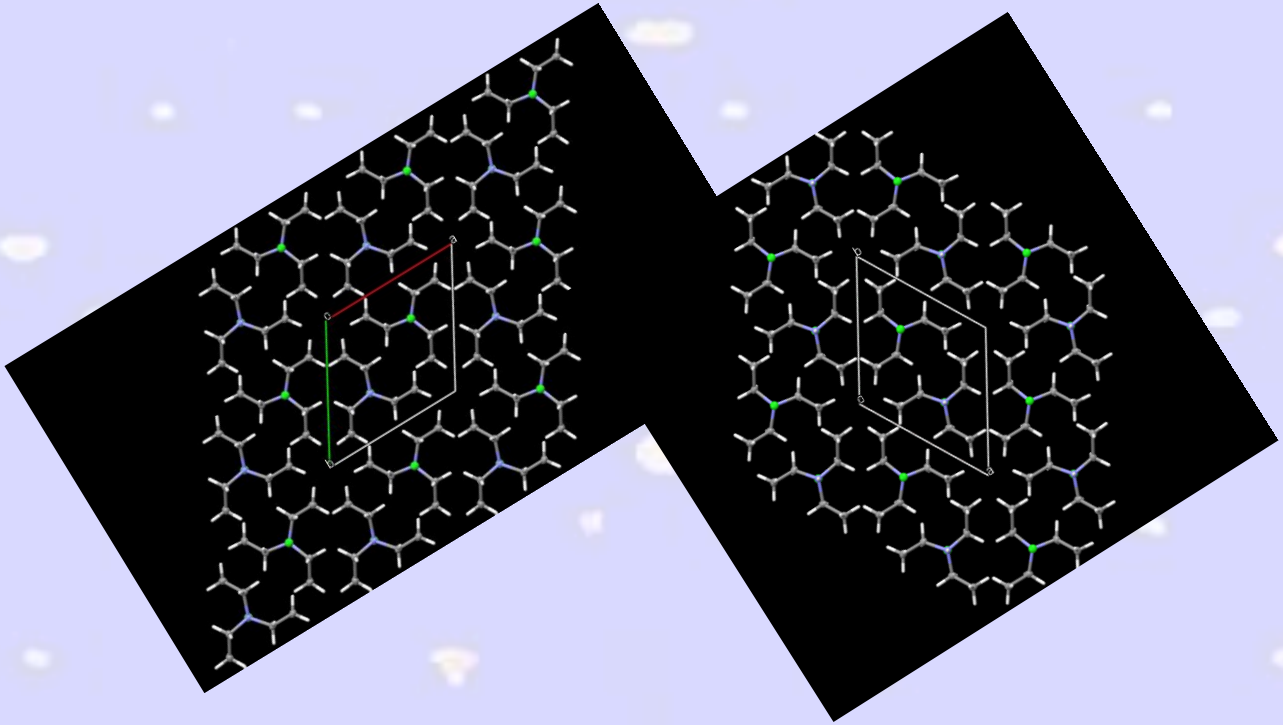




Growth of twin crystal related by the $\begin{pmatrix} -1 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ rotation matrix.



It is not clear which surface of the crystal is acting as the twin interface.

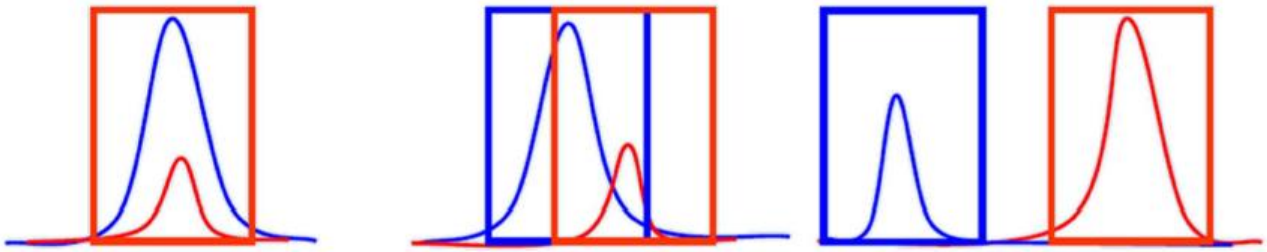


Non-Merohedral Twinning

The twin operator can be represented by an arbitrary operator not related to the Laue Class. It can be a mirror or a 180 degree rotation about a crystal growth surface. There is no exact overlap of diffraction spots and the unit cell may appear too large and not refine well. Spots in the diffraction pattern may be too close or appear split.

George Sheldrick's program 'cell_now' can be used to find multiple crystal orientations and matrices for integration. An HKLF 5 formatted hkl file contains the multiple sets of indices for overlapping reflections. The twinning can be deconvoluted once a structural model is found.

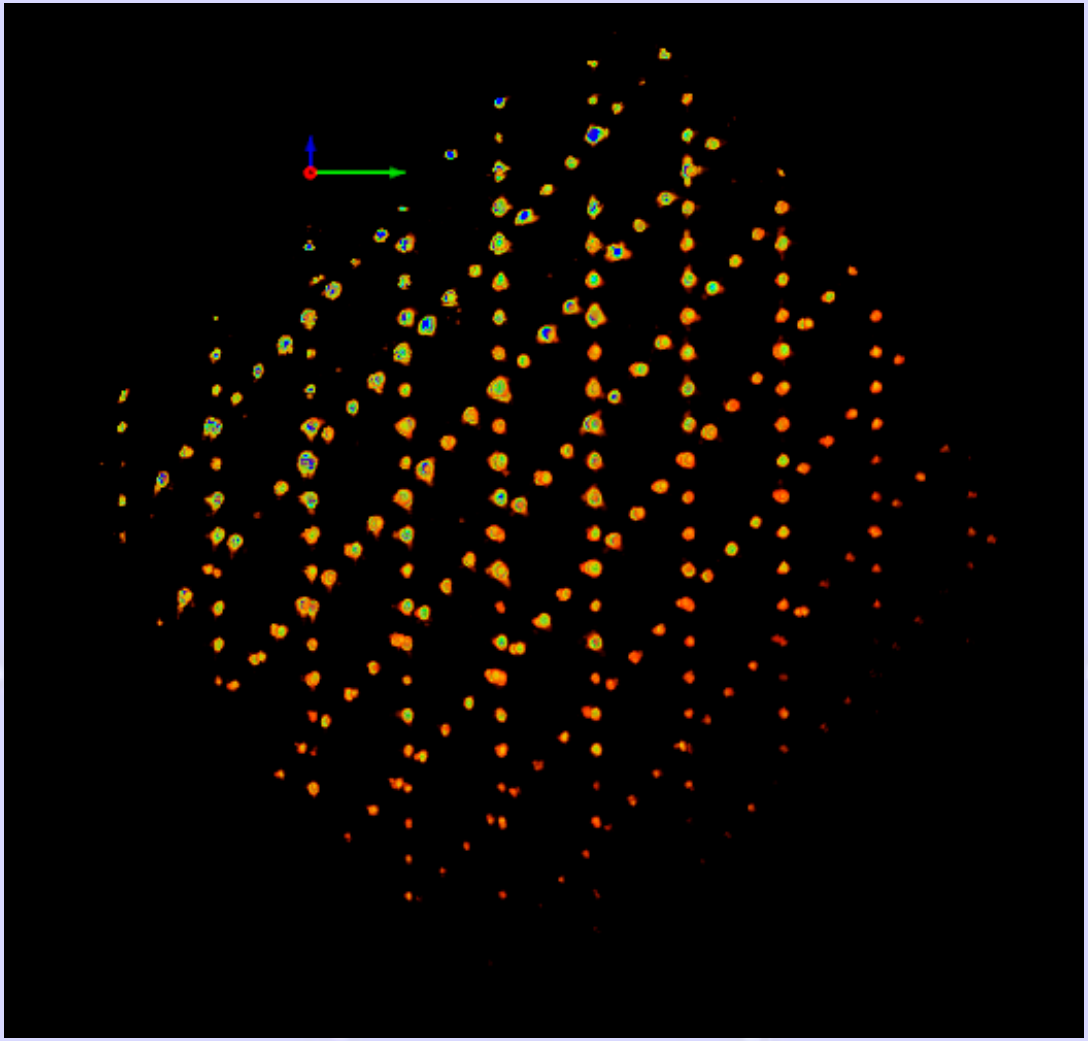
Integration



exact overlaps

partial overlaps

non-overlaps



Diffraction pattern from a non-merohedral twin

Cell Determination

CELL_NOW

- Reads .spin, .p4p or .drx-files
- tries to find sets of reciprocal lattice planes that pass close to as many reflections as possible
- The cell may be rotated to locate further twin domains using only the reflections that have not yet been indexed
- Determination of the cell and the twin law in one program
- Writes a .p4p/.spin file for RLATT and SAINT for simultaneous integration of more than one domain
- Determination of very weak domains possible

Twinning Symptoms

- Not all reflections fit in a single lattice
- Statistics <|E2-1|> small etc.
- Problems to solve the structure
- Poor refinement
- wR2 >> 2 * R1
- Ghost peaks at chemically impossible positions.
- High value of the second Wght parameter
- Fobs >> Fcalc for a large number of reflections
- Etc.

Ton

Ideas behind the Platon's TwinRotMat Algorithm

- Reflections effected by twinning show-up in the least-squares refinement with F(obs) >> F(calc)
- Overlapping reflections necessarily have the same Theta value within a certain tolerance.
- Generate a list of implied possible twin axes based on the above observations.
- Test each proposed twin law for its effect on R.

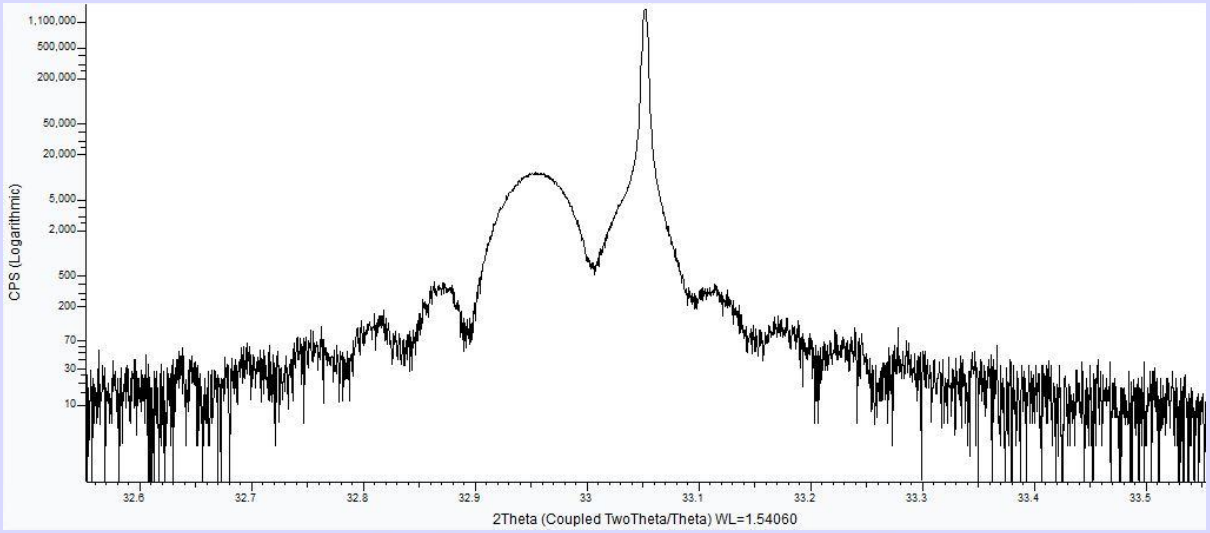
Ton

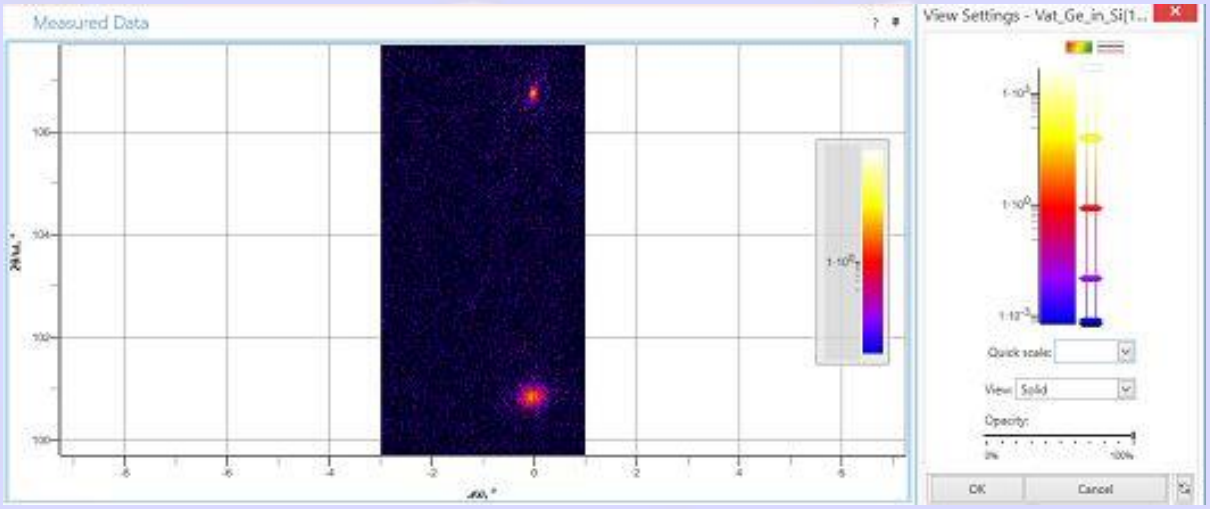
TwinRotMat

- Points to the effective twin laws to be included in the structure refinement given a partially refined structure model
- Offers a diagnostic tool for possibly missed twinning as part crystal structure validation
- Nowadays possibly less important for the detection of non-merohedral twinning (area detectors)

(But cases of missed non-merohedral twinning still arrive for publication)

Ton

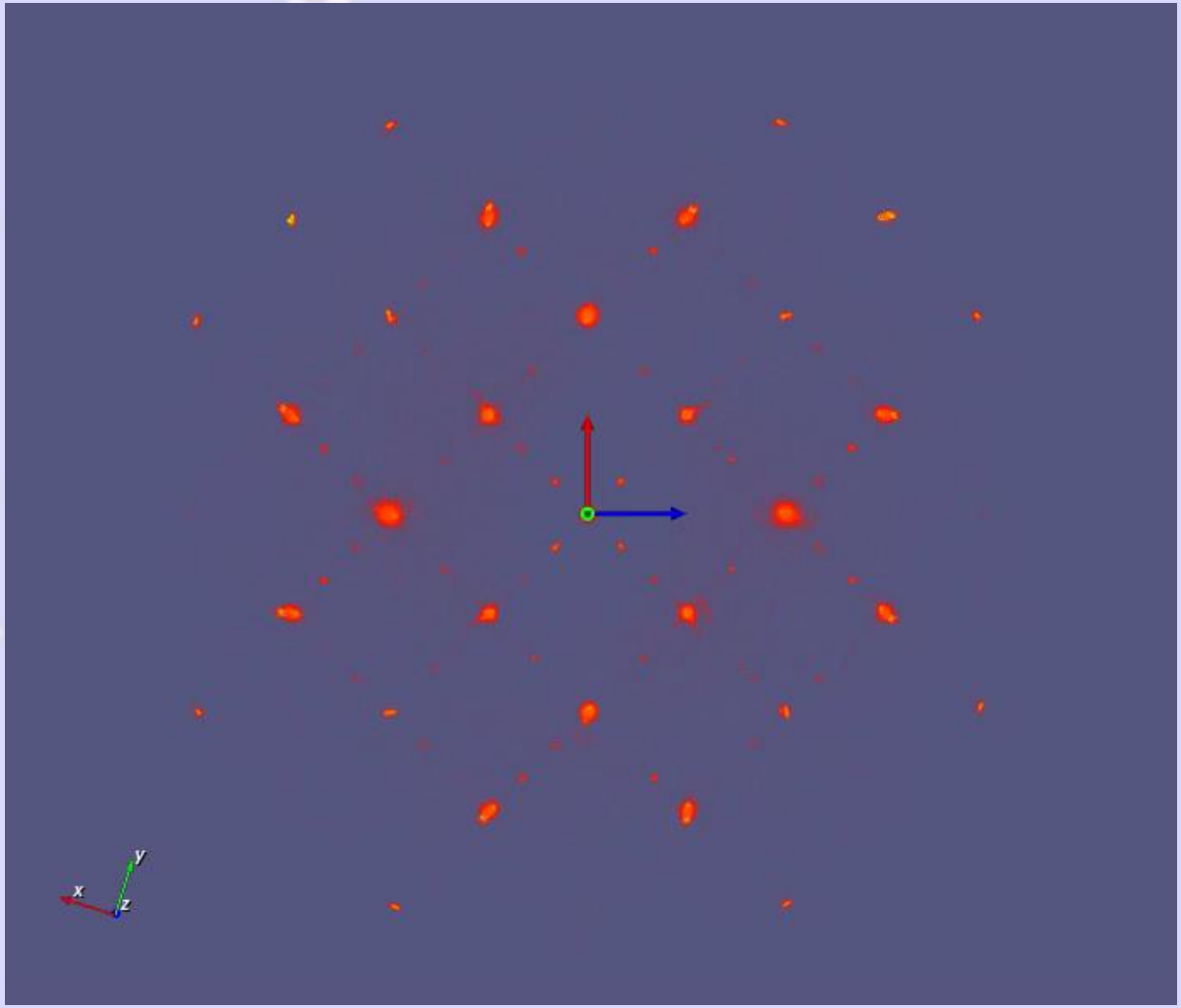




HRXRD quantitative analyses of an epitaxial single crystal thin film on a single crystal substrate. Rigaku SmartLab, sealed tube Cu, 4-bounce Ge, (2-bounce analyzer)

3D diffraction pattern from an epitaxial 25nm thin film of GaAs on a single crystal wafer of something cubic

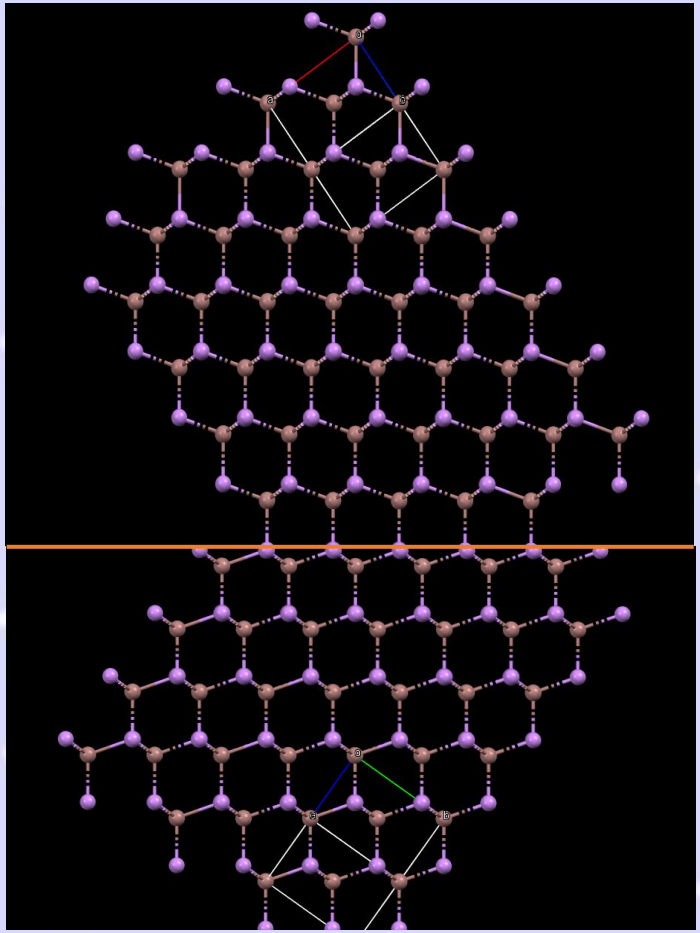
Isolated (111) shell highlighted in yellow



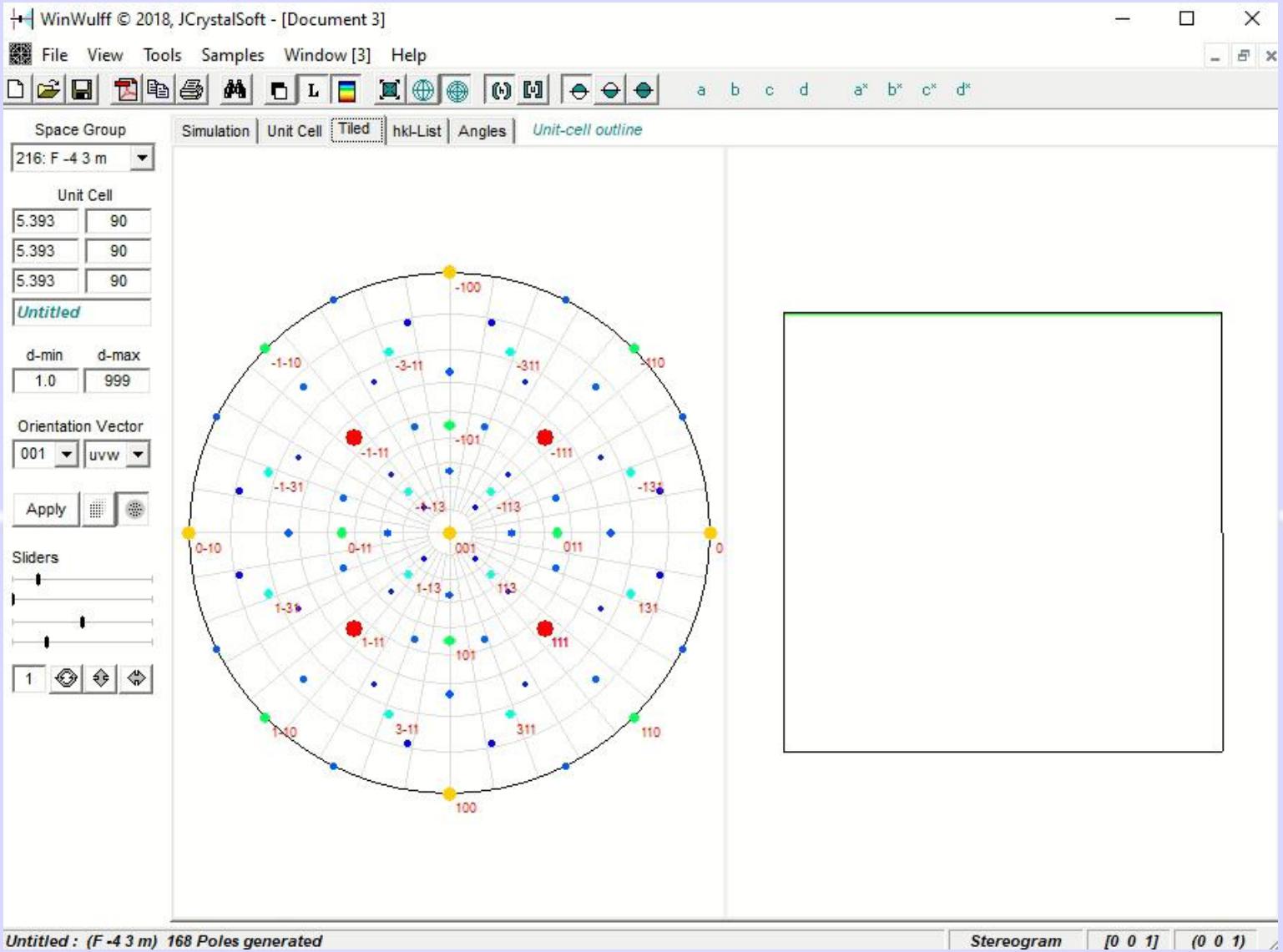
Ryan Lewis and Trevor Smith, McMaster

Growth of a cubic GaAs crystal with a 180° rotation on the (111) face.

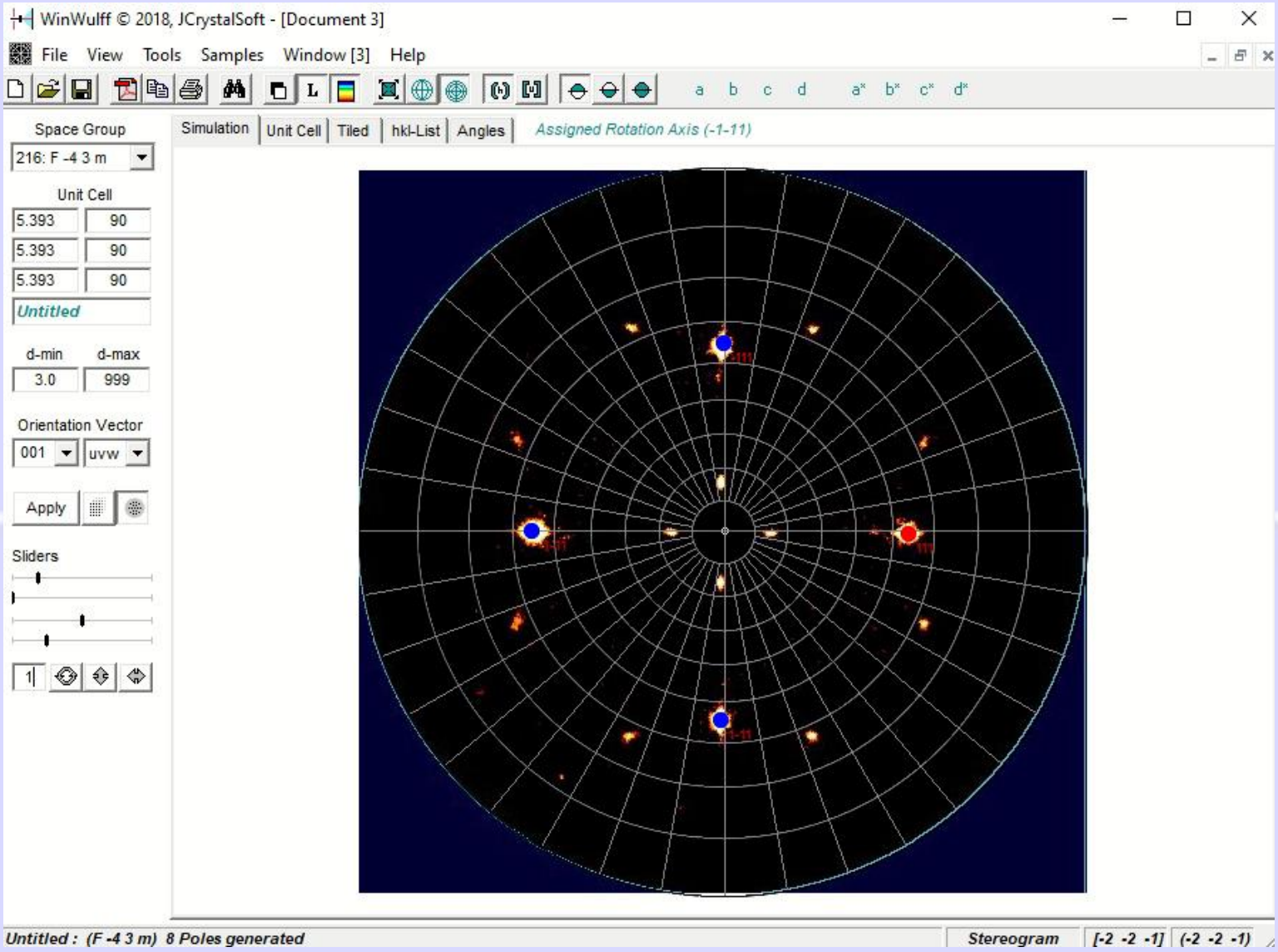
(111) twinning plane →

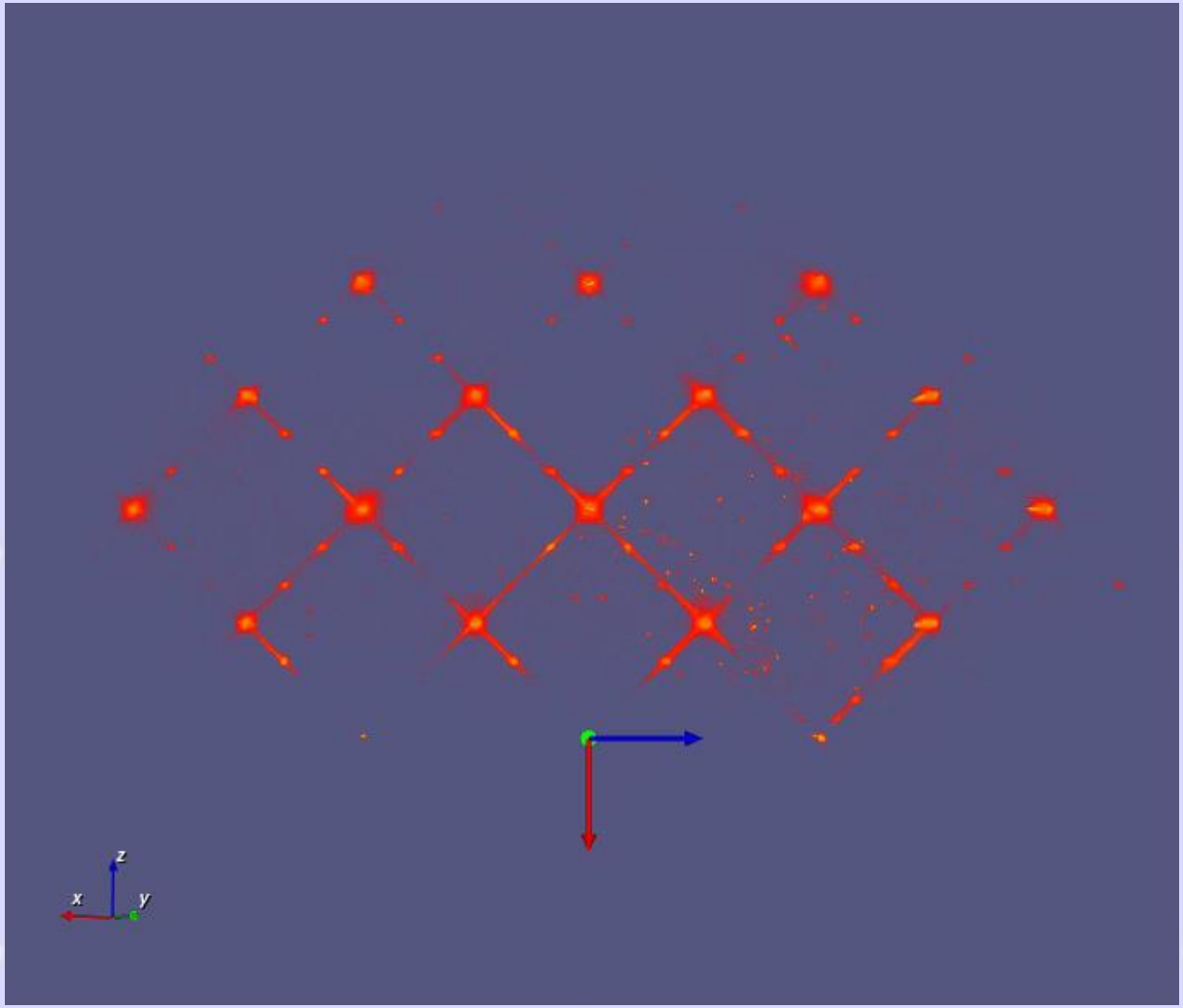


F-43m cube displayed in WinWulff



Simulated 111 twinning (twice) accounts for all crystal orientations





220 nm film of something on GaAs
Bruker Cu IμS, Photon III detector, 7min

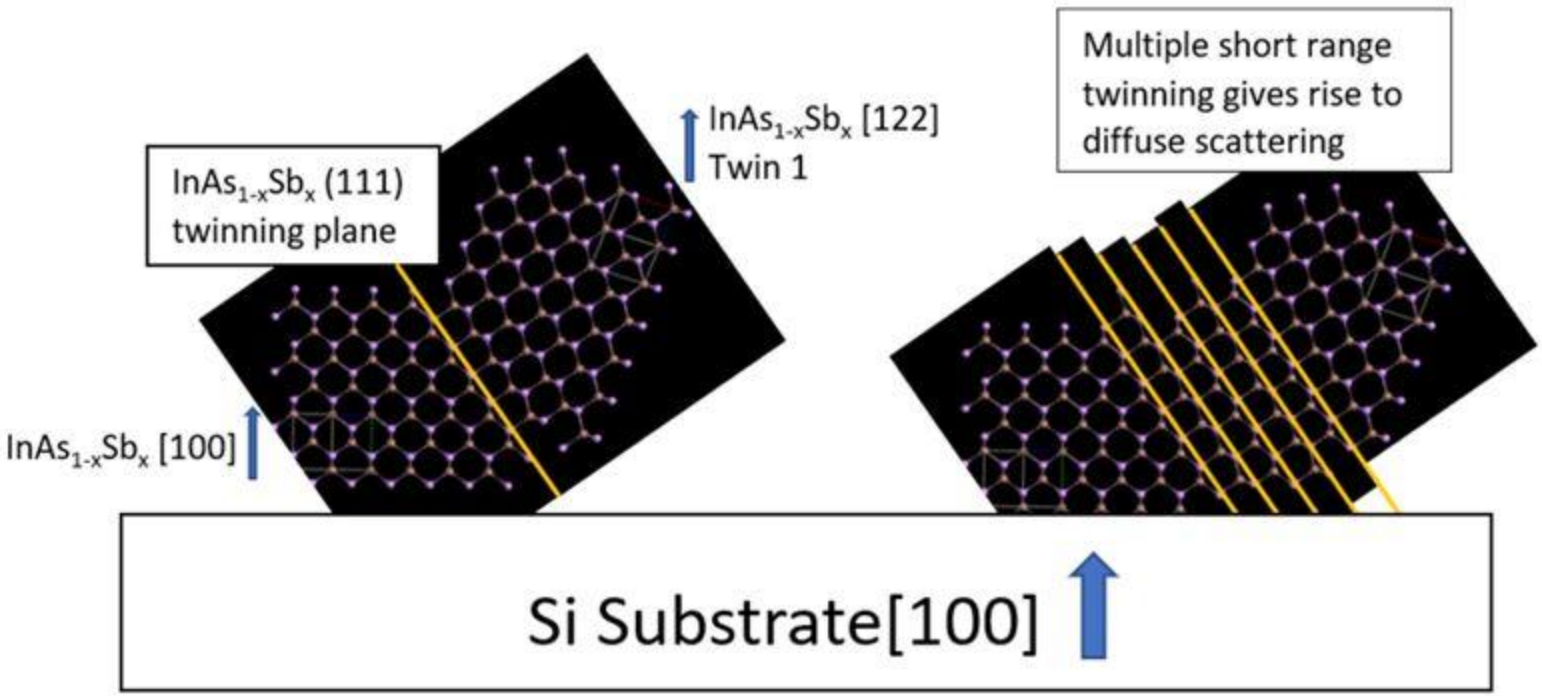


Figure 3. Twinning by 180° (or ±60°) rotation about the [111] face of $InAs_{1-x}Sb_x$. Regions of multiple layer twinning account for the diffuse scattering observed in the 3D diffraction pattern. Twin planes are indicated by yellow lines.

Goosney, Jarvis, Britten, Lapierre, Infrared Physics and Technology

Pseudo-merohedral twinning

The twin operator belongs to a higher crystal system than the true structure.

Metric symmetry appears higher than the Laue symmetry.

McMaster University

Elucidating the structure of the organic spin-liquid candidate k-$(BEDT\text{-}TTF)_2$-Cu_2-$(CN)_3$

Dalini Maharaj
January 29th 2014
Chem 736

- Some physical and crystallographic properties
- Data Collection & Processing
- Refinement in Olex 2
- Discussion of results

Apex 2: Bravais Cell Selection

Final choice

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--------------------------------------------------------------------------------

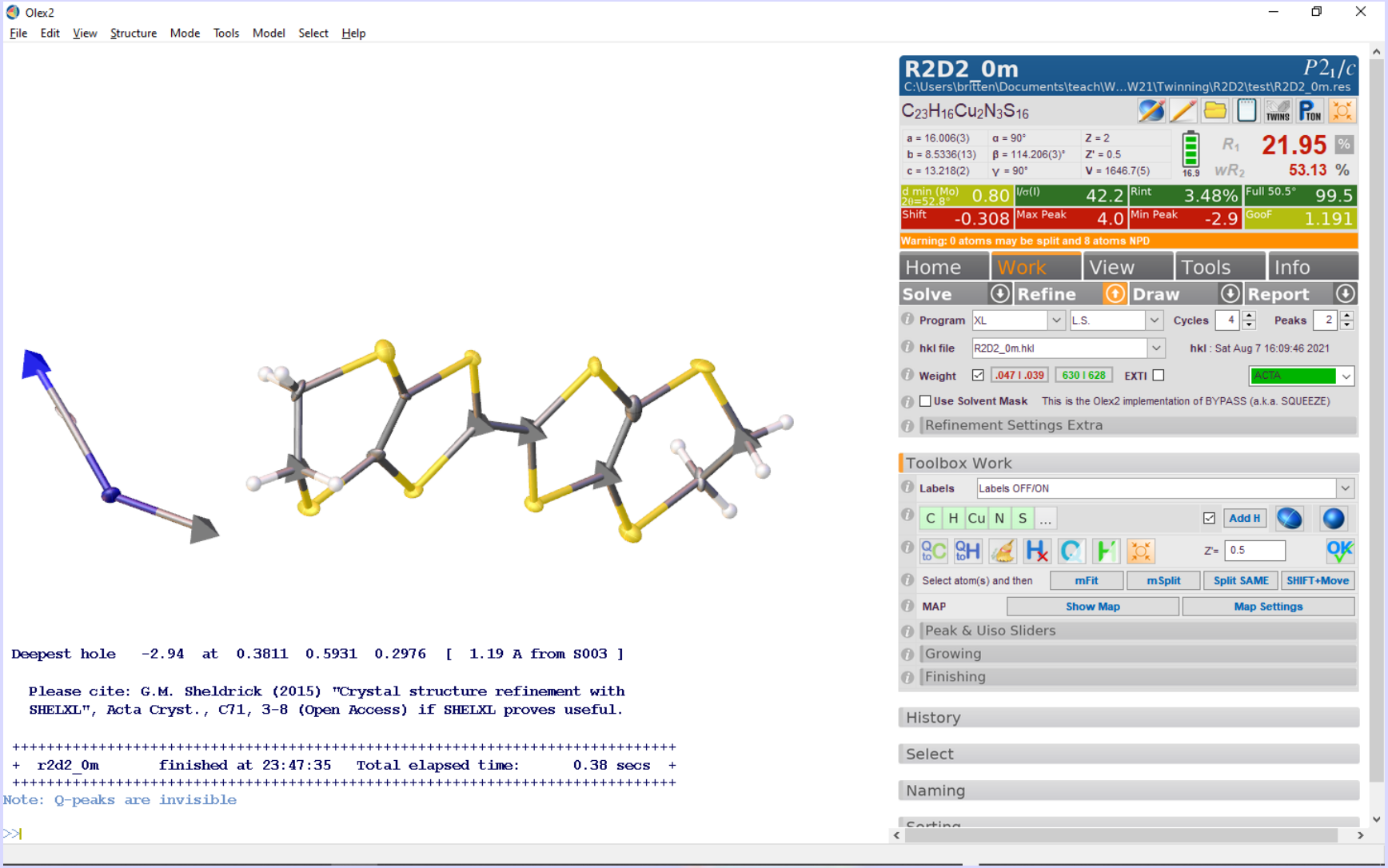
Search for higher metric symmetry
Identical indices and Friedel opposites combined before calculating R(sym)
--------------------------------------------------------------------------------
Option A: FOM = 0.183 deg.   ORTHORHOMBIC C-lattice   R(sym) = 0.198 [   4787]
Cell:    13.218  29.197   8.534   90.00   90.00   89.82     Volume:      3293.44
Matrix: 0.0000  0.0000 -1.0000 -2.0000  0.0000 -1.0000  0.0000  1.0000  0.0000
--------------------------------------------------------------------------------
Option B: FOM = 0.000 deg.   MONOCLINIC   P-lattice   R(sym) = 0.016 [   3111]
Cell:    13.218   8.534  16.006   90.00  114.21   90.00     Volume:      1646.72
Matrix: 0.0000  0.0000 -1.0000  0.0000 -1.0000  0.0000 -1.0000  0.0000  0.0000
--------------------------------------------------------------------------------
Option C: FOM = 0.182 deg.   MONOCLINIC   C-lattice   R(sym) = 0.208 [   3178]
Cell:    29.197  13.218   8.534   90.00   90.00   90.18     Volume:      3293.44
Matrix: 2.0000  0.0000  1.0000  0.0000  0.0000 -1.0000  0.0000  1.0000  0.0000
--------------------------------------------------------------------------------
Option D: FOM = 0.183 deg.   MONOCLINIC   C-lattice   R(sym) = 0.203 [   3255]
Cell:    13.218  29.197   8.534   90.00   90.00   89.82     Volume:      3293.44
Matrix: 0.0000  0.0000  1.0000  2.0000  0.0000  1.0000  0.0000  1.0000  0.0000

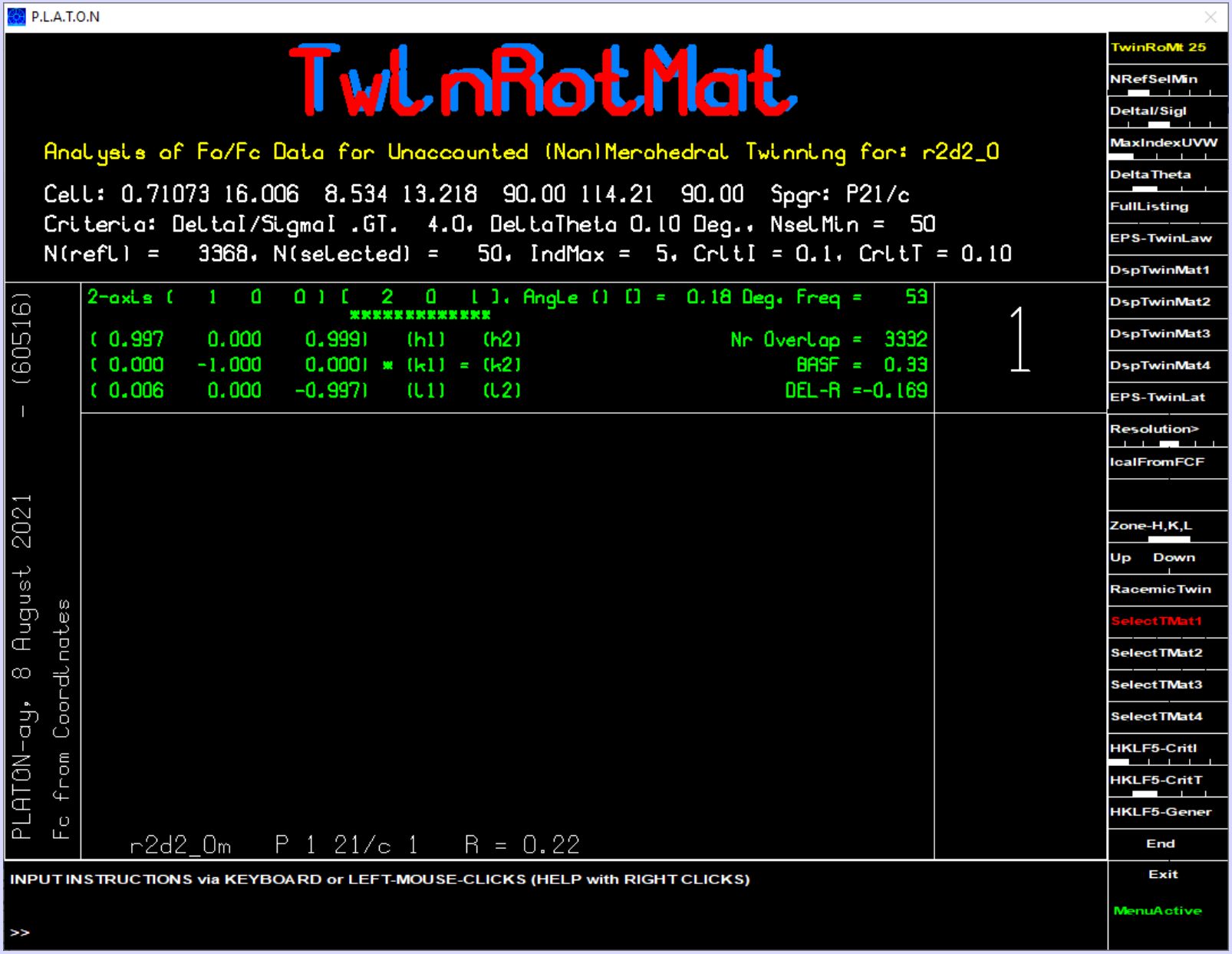
Current cell not changed

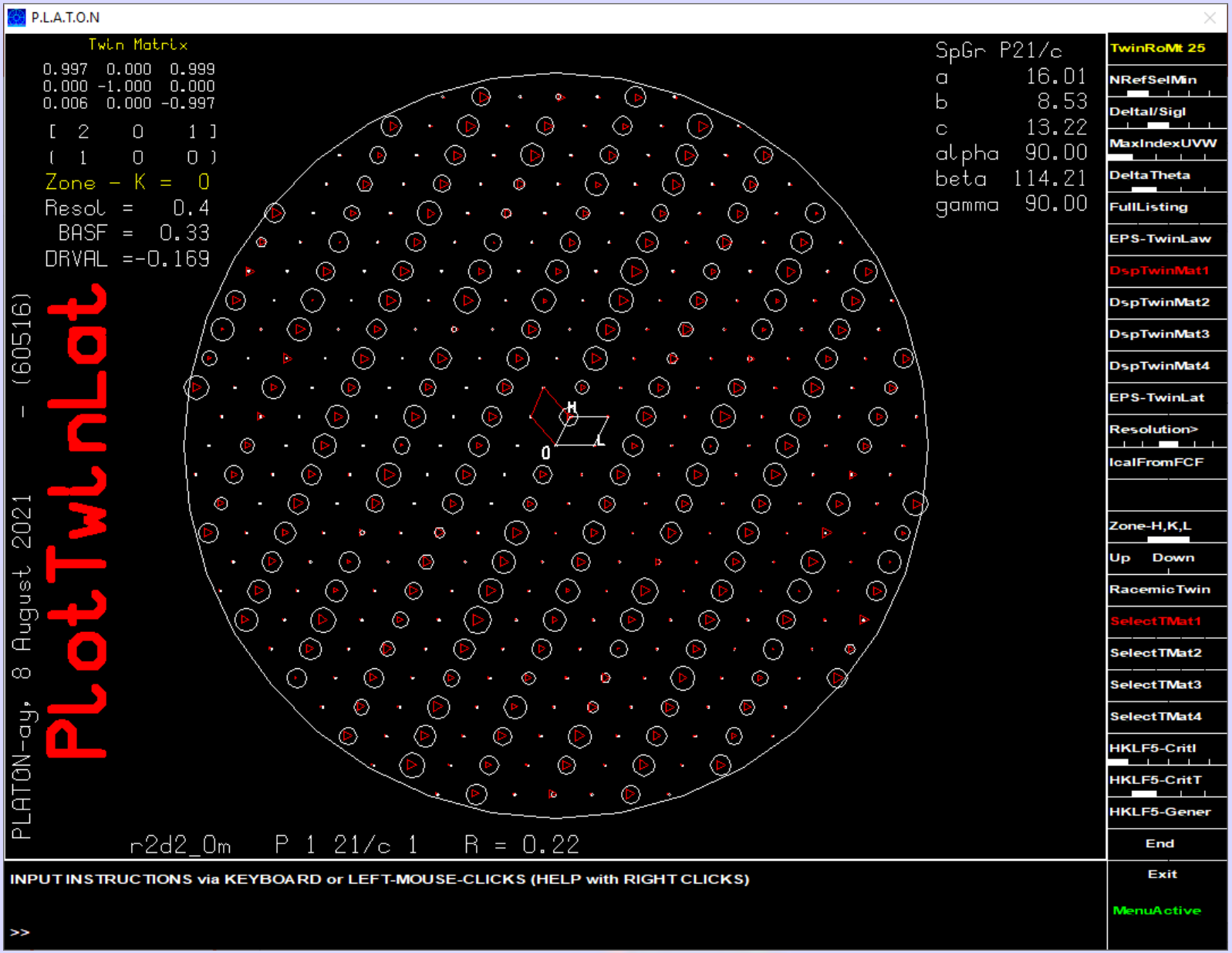
--------------------------------------------------------------------------------
```

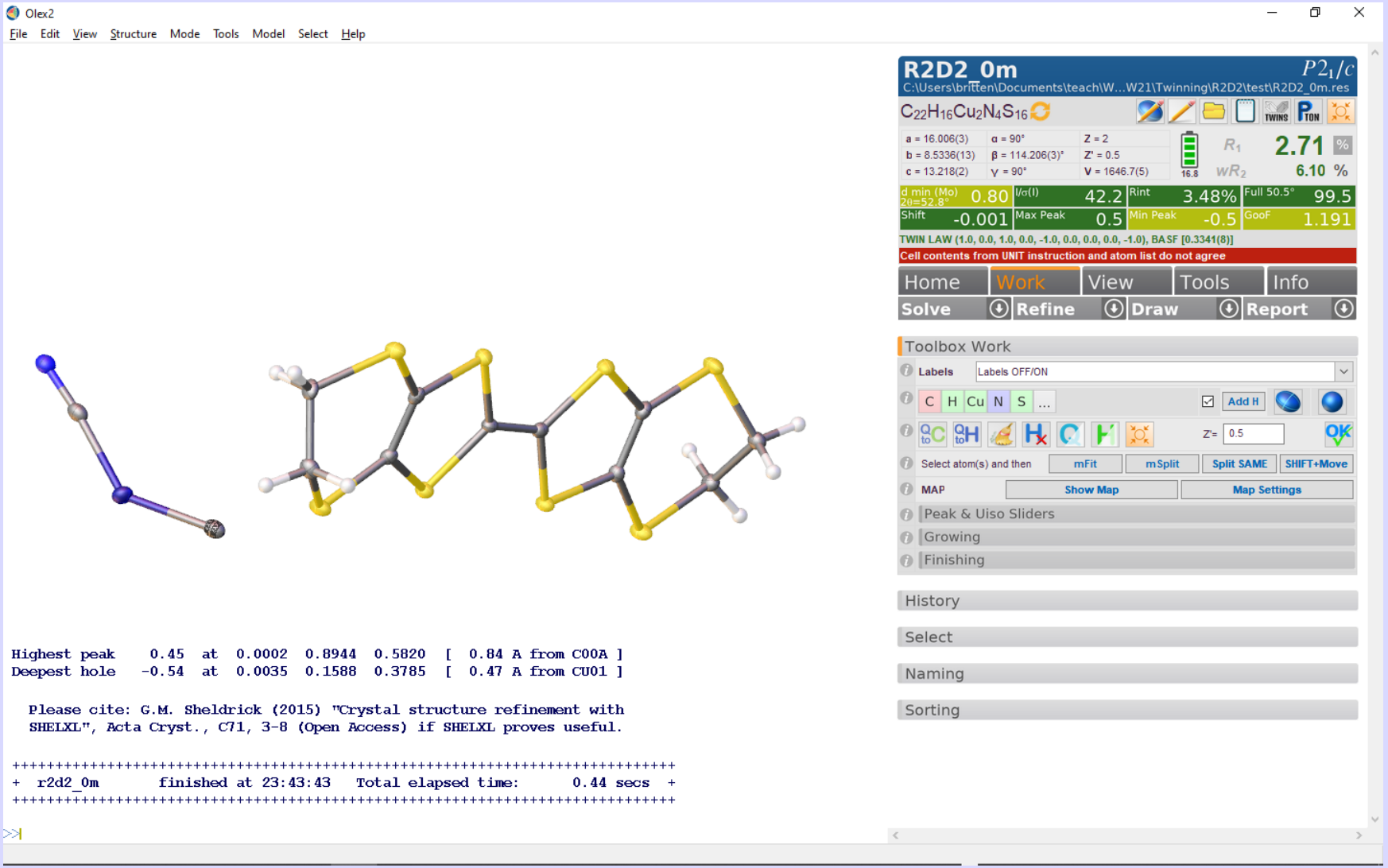
Fig 6: Possible space groups obtained from .prp file

Relatively small R values for other possibilities

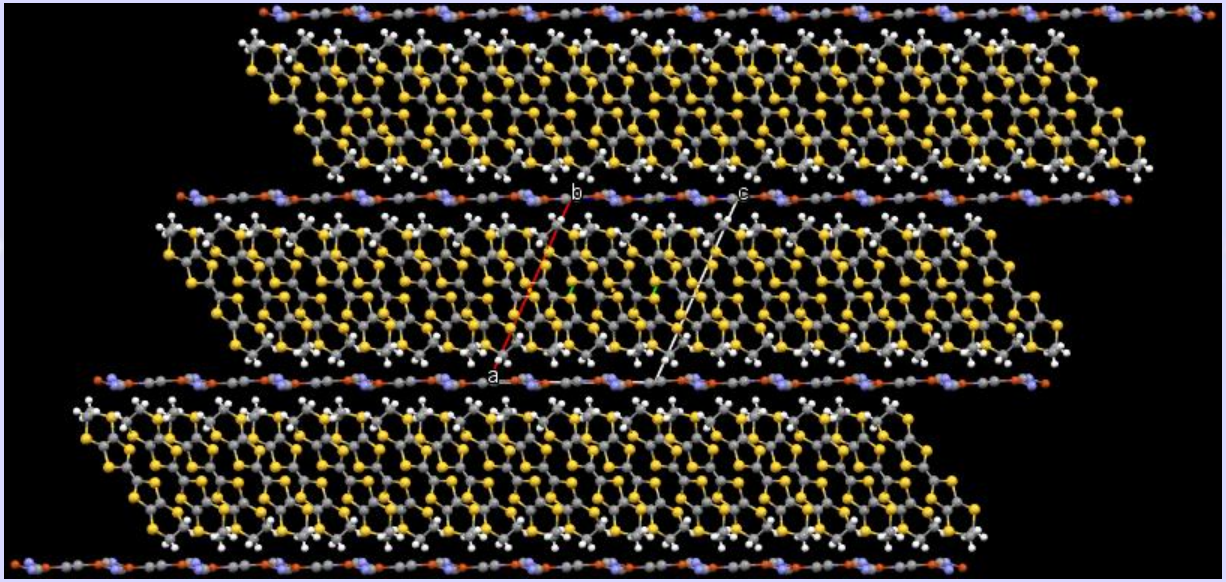

Olex2
File Edit View Structure Mode Tools Model Select Help
R2D2_0m
P2₁/c
C:\Users\britten\Documents\teach\W...W21\Twinning\R2D2\test\R2D2_0m.res
C23H16Cu2N3S16
a = 16.006(3) α = 90° Z = 2
b = 8.5336(13) β = 114.206(3)° Z' = 0.5
c = 13.218(2) γ = 90° V = 1646.7(5)
16.9
R1 21.95 %
wR2 53.13 %
d min (Mo) 0.80
2θ=52.8°
I/σ(I) 42.2
Rint 3.48%
Full 50.5° 99.5
Shift -0.308
Max Peak 4.0
Min Peak -2.9
GooF 1.191
Warning: 0 atoms may be split and 8 atoms NPD
Home Work View Tools Info
Solve Refine Draw Report
Program XL L.S. Cycles 4 Peaks 2
hkl file R2D2_0m.hkl hkl : Sat Aug 7 16:09:46 2021
Weight .047 I .039 630 I 628 EXTI ACTA
Use Solvent Mask This is the Olex2 implementation of BYPASS (a.k.a. SQUEEZE)
Refinement Settings Extra
Toolbox Work
Labels Labels OFF/ON
C H Cu N S ...
Add H
Z'= 0.5
Select atom(s) and then mFit mSplit Split SAME SHIFT+Move
MAP Show Map Map Settings
Peak & Uiso Sliders
Growing
Finishing
History
Select
Naming
Deepest hole -2.94 at 0.3811 0.5931 0.2976 [1.19 A from S003]
Please cite: G.M. Sheldrick (2015) "Crystal structure refinement with SHELXL", Acta Cryst., C71, 3-8 (Open Access) if SHELXL proves useful.
+ r2d2_0m finished at 23:47:35 Total elapsed time: 0.38 secs +
Note: Q-peaks are invisible
>>


P.L.A.T.O.N
TwinRotMat
Analysis of Fo/Fc Data for Unaccounted (Non)Merohedral Twinning for: r2d2_0
Cell: 0.71073 16.006 8.534 13.218 90.00 114.21 90.00 Spgr: P21/c
Criteria: DeltaI/SigmaI .GT. 4.0, DeltaTheta 0.10 Deg., NselMin = 50
N(refl) = 3368, N(selected) = 50, IndMax = 5, CrltI = 0.1, CrltT = 0.10
2-axis (1 0 0) [2 0 1], Angle () [] = 0.18 Deg, Freq = 53
(0.997 0.000 0.999) (h1) (h2) Nr Overlap = 3332
(0.000 -1.000 0.000) * (k1) = (k2) BASF = 0.33
(0.006 0.000 -0.997) (l1) (l2) DEL-R =-0.169
1
PLATON-ay, 8 August 2021 - (60516)
Fc from Coordinates
r2d2_0m P 1 21/c 1 R = 0.22
INPUT INSTRUCTIONS via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>
TwinRoMt 25
NRefSelMin
DeltaI/SigI
MaxIndexUVW
DeltaTheta
FullListing
EPS-TwinLaw
DspTwinMat1
DspTwinMat2
DspTwinMat3
DspTwinMat4
EPS-TwinLat
Resolution>
IcalFromFCF
Zone-H,K,L
Up Down
RacemicTwin
SelectTMat1
SelectTMat2
SelectTMat3
SelectTMat4
HKLF5-CritI
HKLF5-CritT
HKLF5-Gener
End
Exit
MenuActive

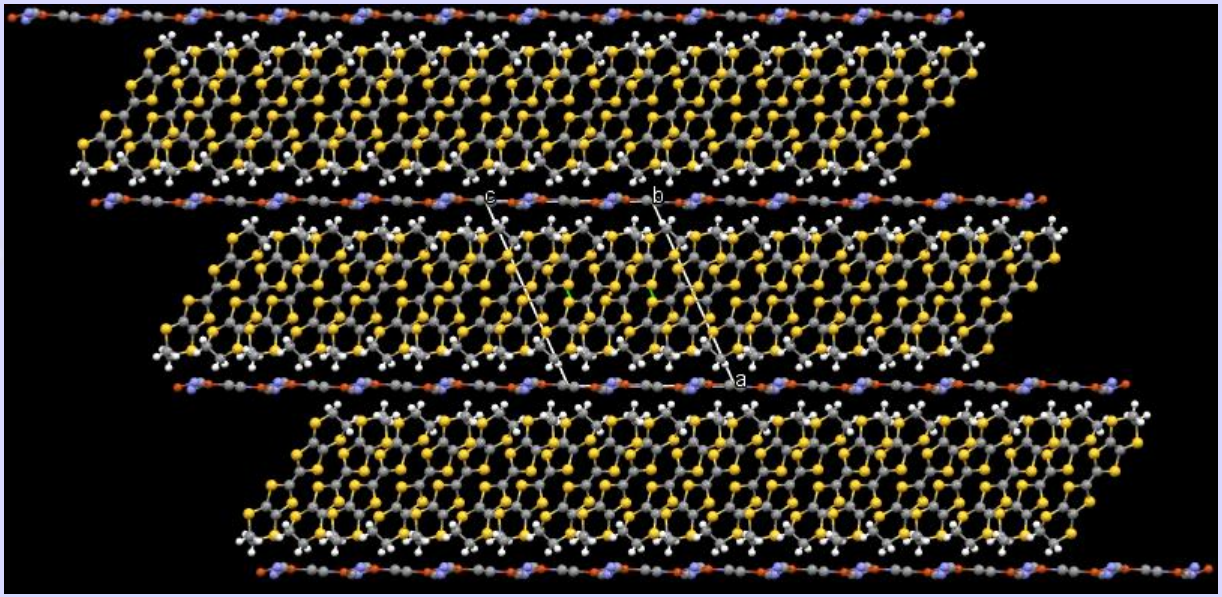

P.L.A.T.O.N
Twin Matrix
0.997 0.000 0.999
0.000 -1.000 0.000
0.006 0.000 -0.997
[2 0 1]
(1 0 0)
Zone - K = 0
Resol = 0.4
BASF = 0.33
DRVAL =-0.169
SpGr P21/c
a 16.01
b 8.53
c 13.22
alpha 90.00
beta 114.21
gamma 90.00
PLATON-ay, 8 August 2021 - (60516)
PlotTwLnLat
H
O
L
r2d2_0m P 1 21/c 1 R = 0.22
TwinRoMt 25
NRefSelMin
DeltaI/SigI
MaxIndexUVW
DeltaTheta
FullListing
EPS-TwinLaw
DspTwinMat1
DspTwinMat2
DspTwinMat3
DspTwinMat4
EPS-TwinLat
Resolution>
IcalFromFCF
Zone-H,K,L
Up Down
RacemicTwin
SelectTMat1
SelectTMat2
SelectTMat3
SelectTMat4
HKLF5-CritI
HKLF5-CritT
HKLF5-Gener
End
Exit
MenuActive
INPUT INSTRUCTIONS via KEYBOARD or LEFT-MOUSE-CLICKS (HELP with RIGHT CLICKS)
>>


Olex2
File Edit View Structure Mode Tools Model Select Help
R2D2_0m
P2₁/c
C:\Users\britten\Documents\teach\W...W21\Twinning\R2D2\test\R2D2_0m.res
C22H16Cu2N4S16
a = 16.006(3)
b = 8.5336(13)
c = 13.218(2)
α = 90°
β = 114.206(3)°
γ = 90°
Z = 2
Z' = 0.5
V = 1646.7(5)
16.8
R1 2.71 %
wR2 6.10 %
d min (Mo) 2θ=52.8° 0.80
I/σ(I) 42.2
Rint 3.48%
Full 50.5° 99.5
Shift -0.001
Max Peak 0.5
Min Peak -0.5
GooF 1.191
TWIN LAW (1.0, 0.0, 1.0, 0.0, -1.0, 0.0, 0.0, 0.0, -1.0), BASF [0.3341(8)]
Cell contents from UNIT instruction and atom list do not agree
Home Work View Tools Info
Solve Refine Draw Report
Toolbox Work
Labels Labels OFF/ON
C H Cu N S ...
Add H
Z'= 0.5
Select atom(s) and then mFit mSplit Split SAME SHIFT+Move
MAP Show Map Map Settings
Peak & Uiso Sliders
Growing
Finishing
History
Select
Naming
Sorting
Highest peak 0.45 at 0.0002 0.8944 0.5820 [0.84 A from C00A]
Deepest hole -0.54 at 0.0035 0.1588 0.3785 [0.47 A from CU01]
Please cite: G.M. Sheldrick (2015) "Crystal structure refinement with SHELXL", Acta Cryst., C71, 3-8 (Open Access) if SHELXL proves useful.
+ r2d2_0m finished at 23:43:43 Total elapsed time: 0.44 secs +

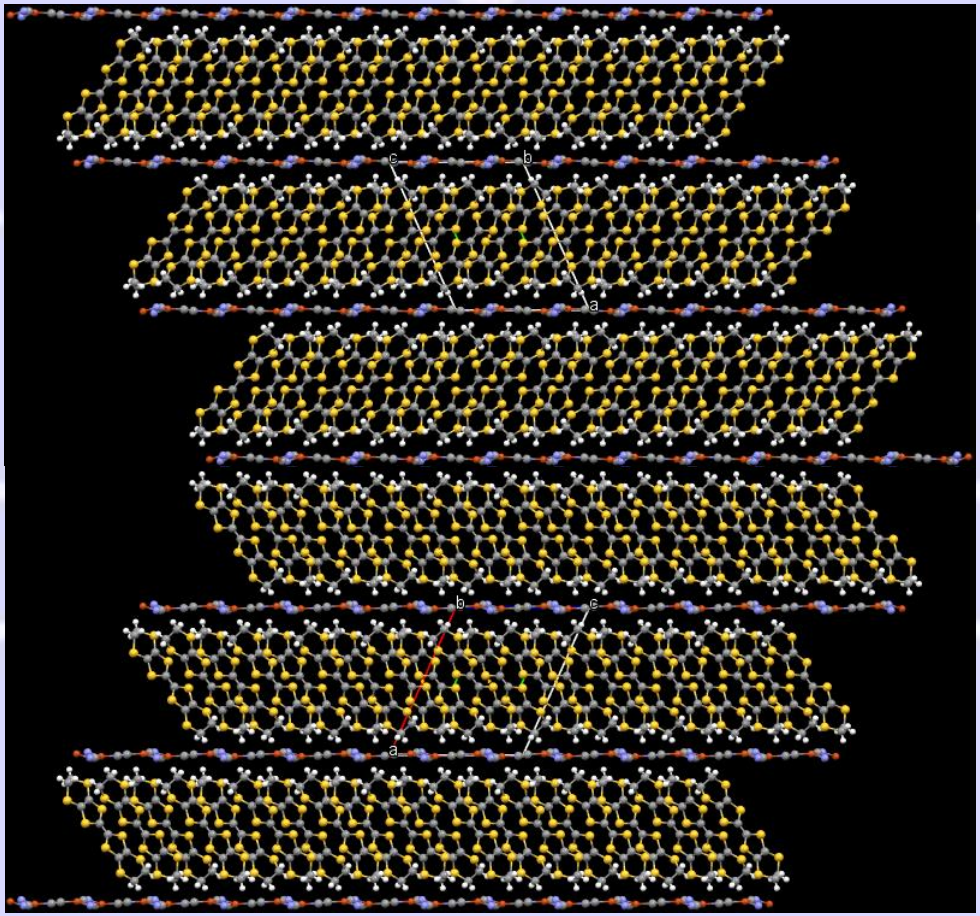
Packing in Dalini's crystal



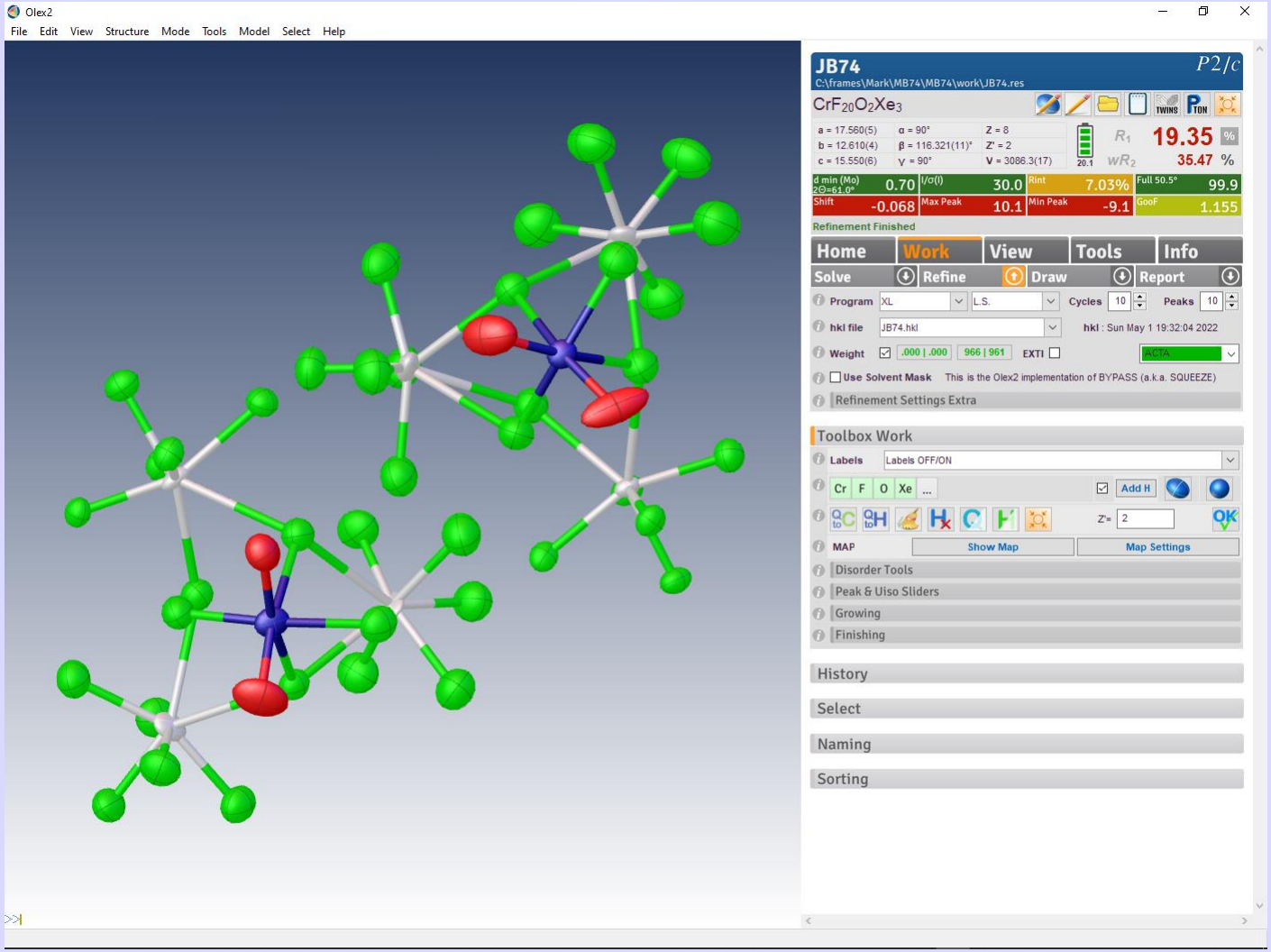
Crystal rotated 180° around **a***



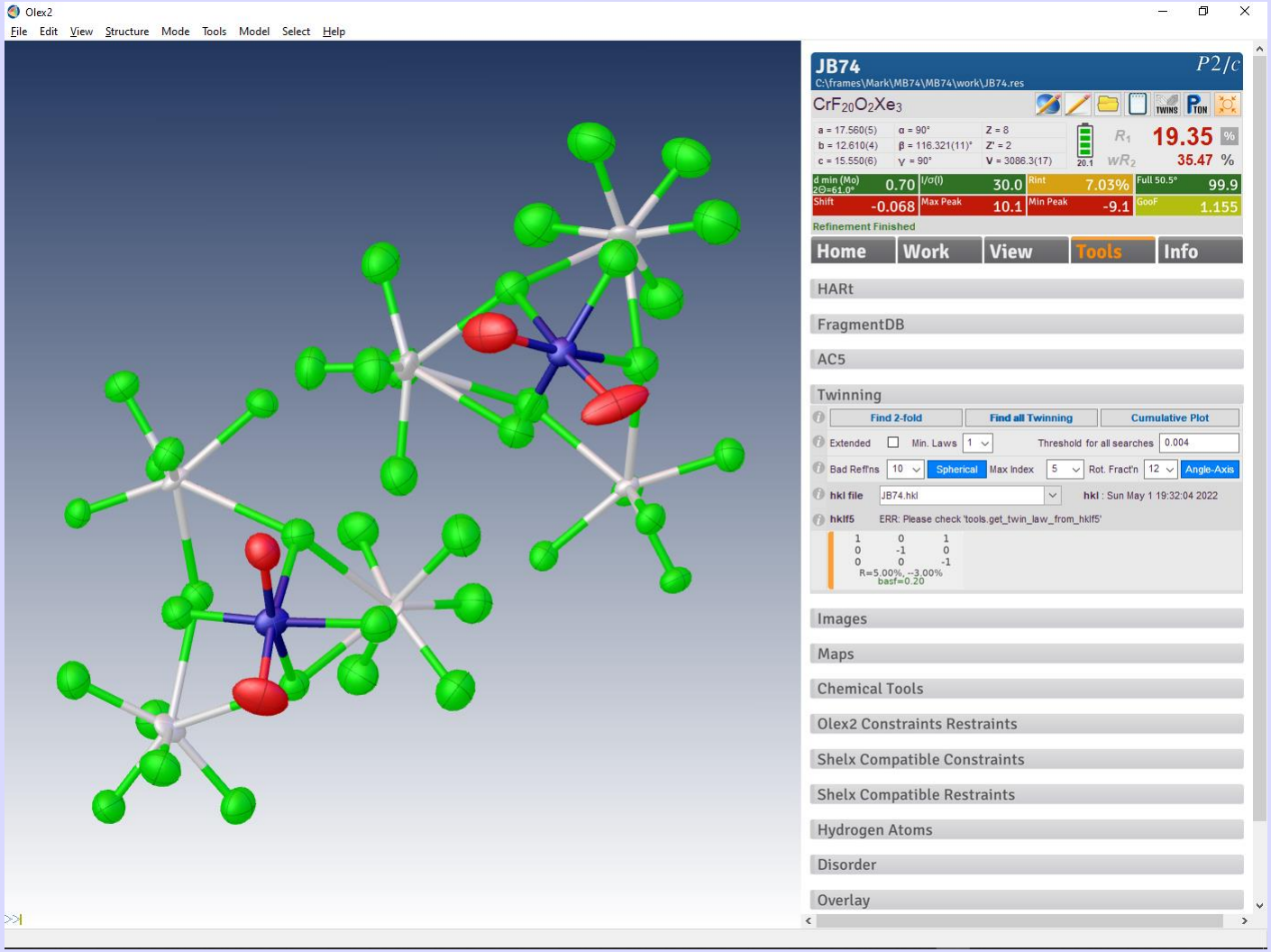
Twinned growth



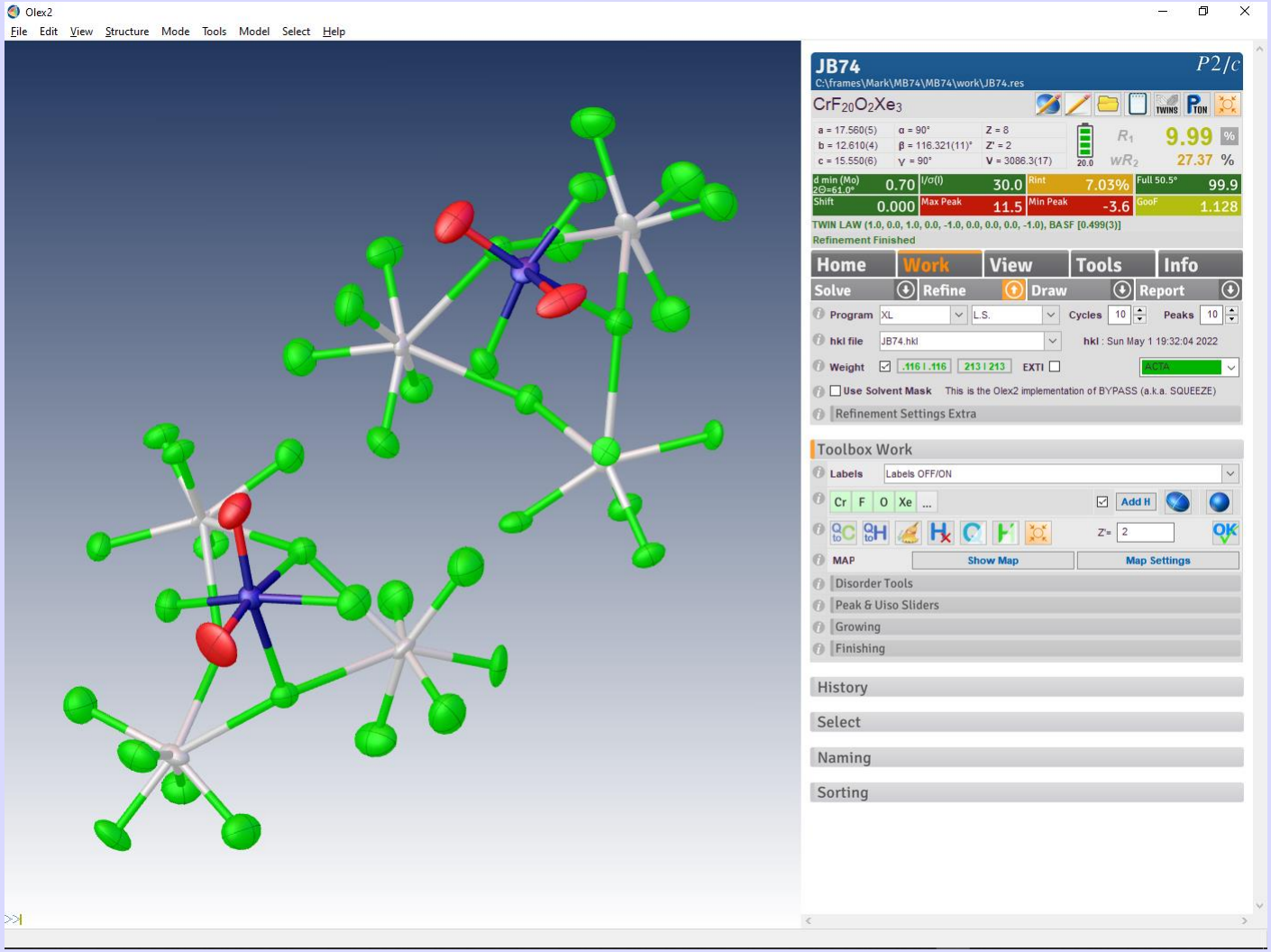
$CrF_{20}O_2Xe_3$ – Schrobilgen, Bortolus



$CrF_{20}O_2Xe_3$ – Schrobilgen, Bortolus

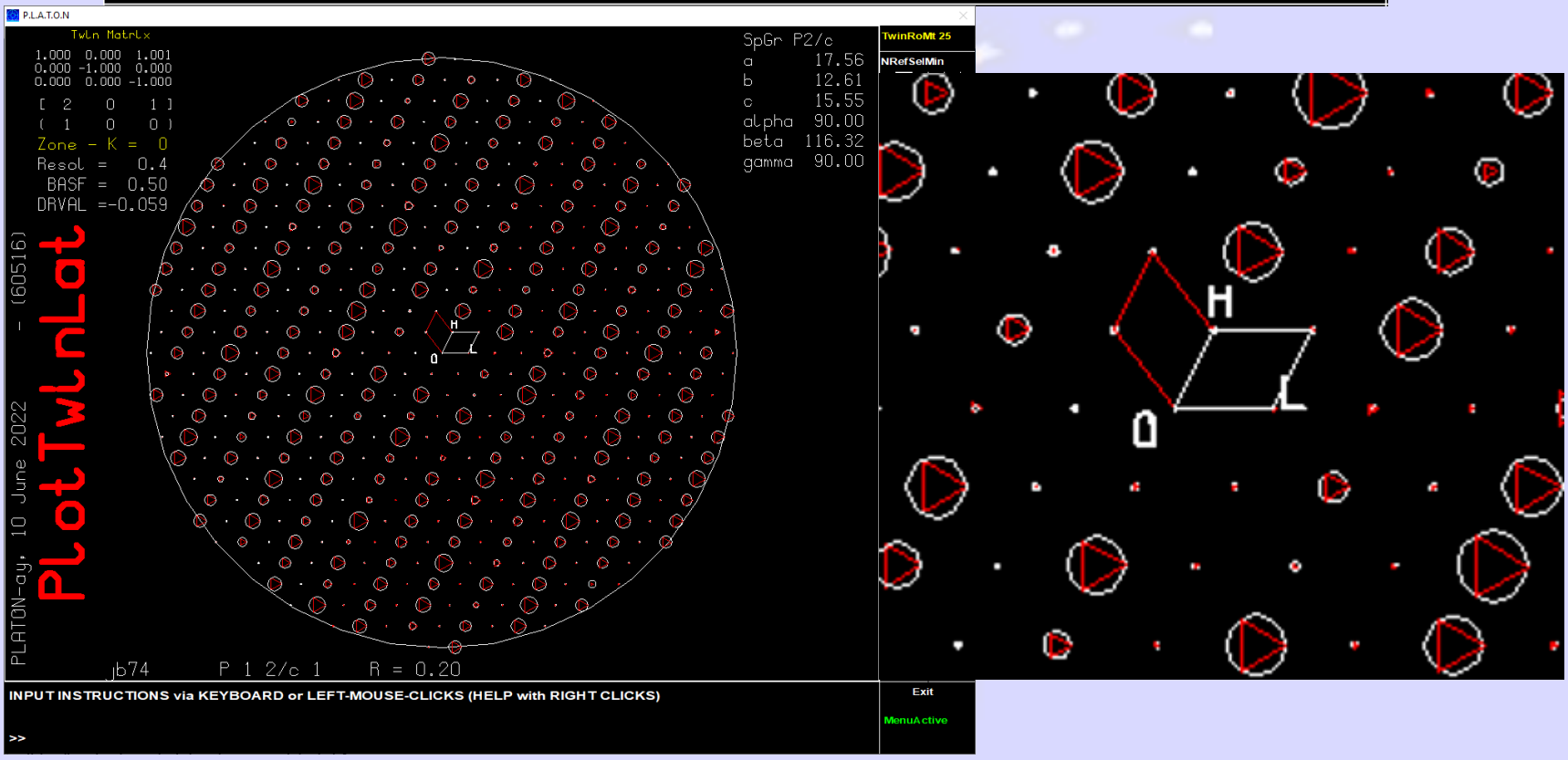


TWIN 1 0 1 0 -1 0 0 0 -1 2

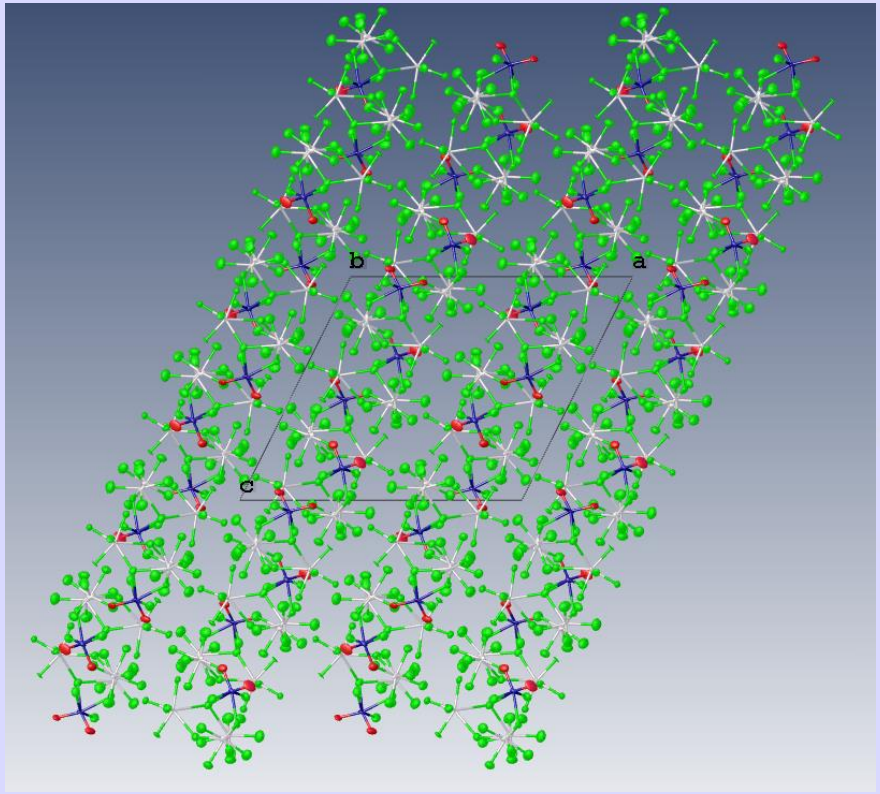


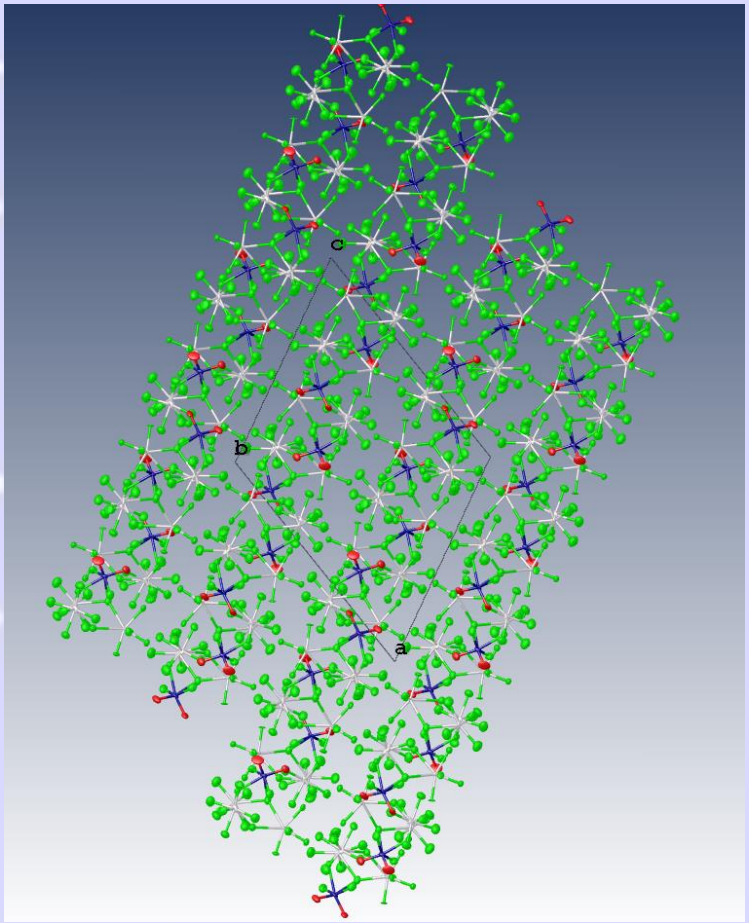
TwinRotMat

```
2-axis (   1    0    0 ) [   2    0    1 ], Angle () [] =   0.04 Deg, Freq =    64
          **************
( 1.000    0.000    1.001)   (h1)   (h2)                  Nr Overlap =  9408
( 0.000   -1.000    0.000) * (k1) = (k2)                  BASF =  0.50
( 0.000    0.000   -1.000)   (l1)   (l2)                  DEL-R =-0.059
```

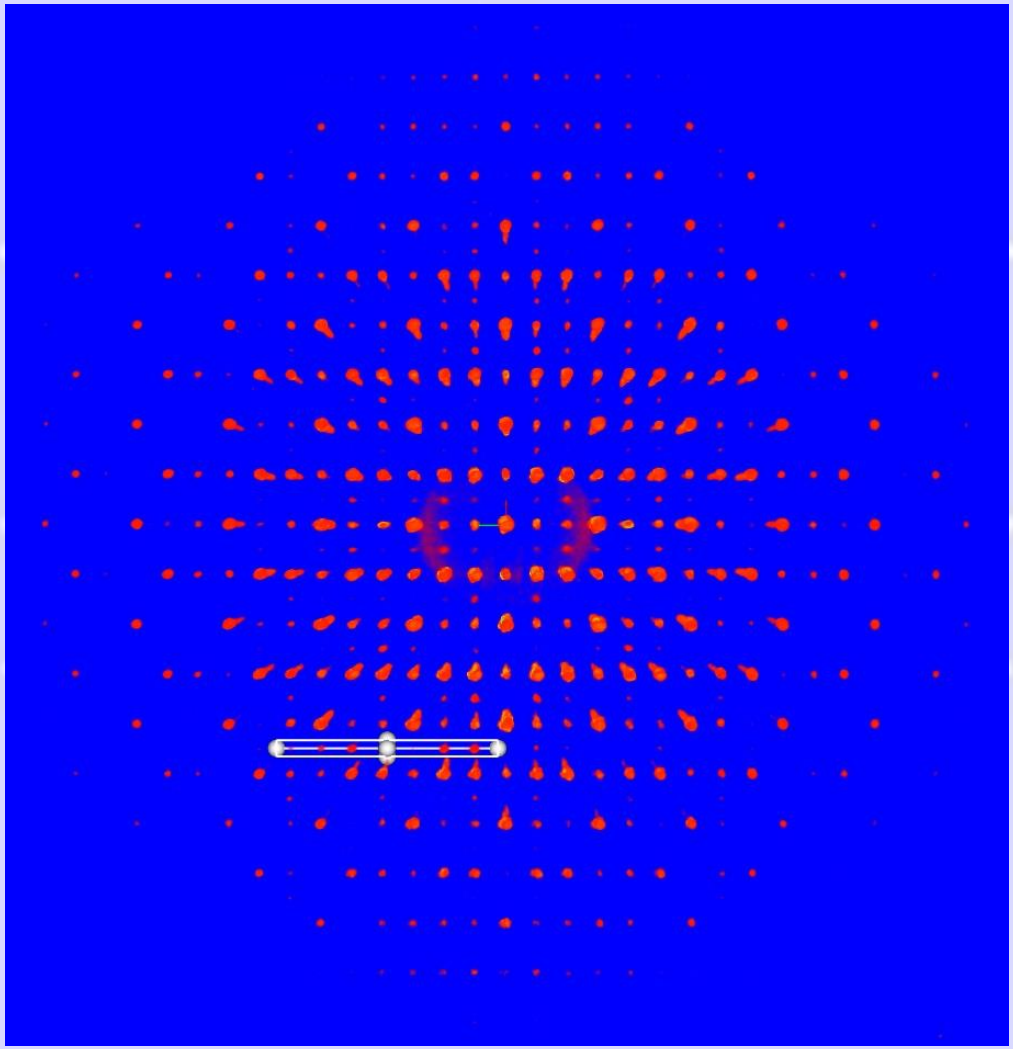


Flip around body diagonal

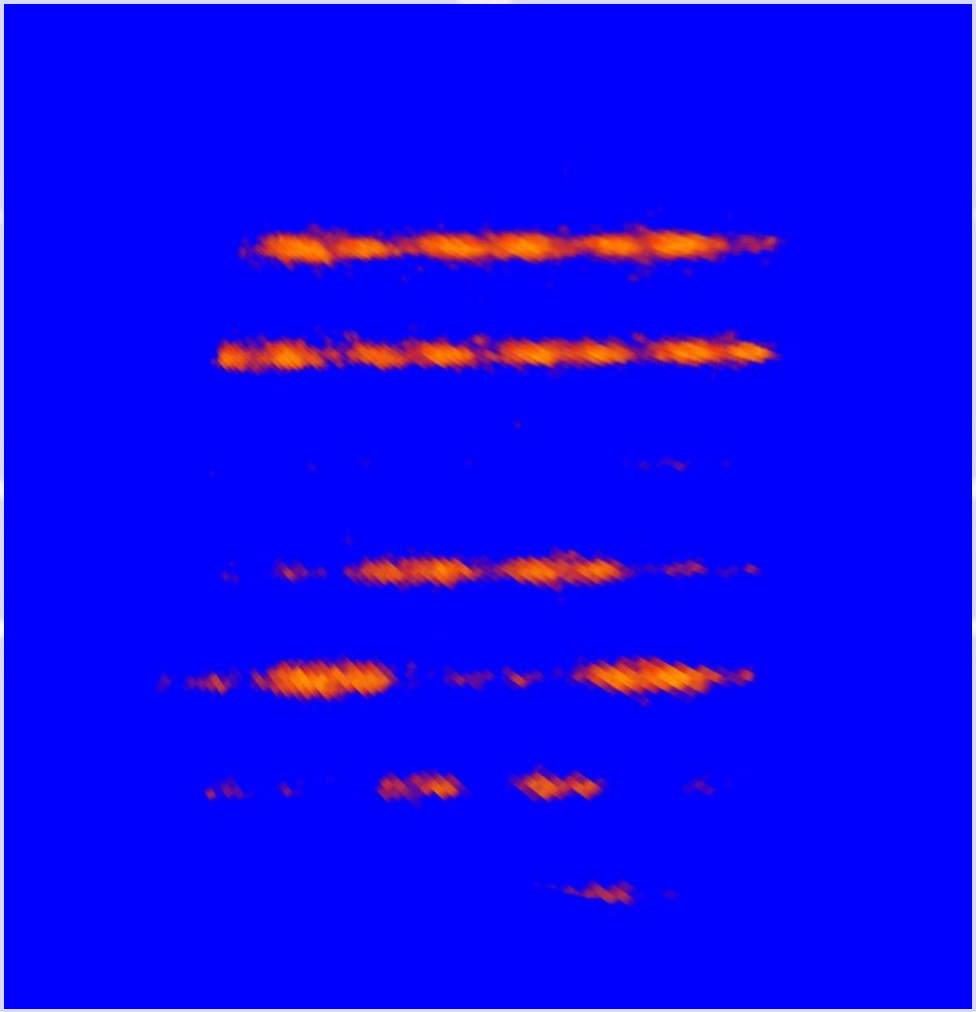




Strong and weak layer in RS



Diffuse scattering, loss of order in 1D



Twinning that isn't twinning

There is no twin operator, but there are 2 or more crystal orientations. The components are not related by any mathematical rule or twin law.

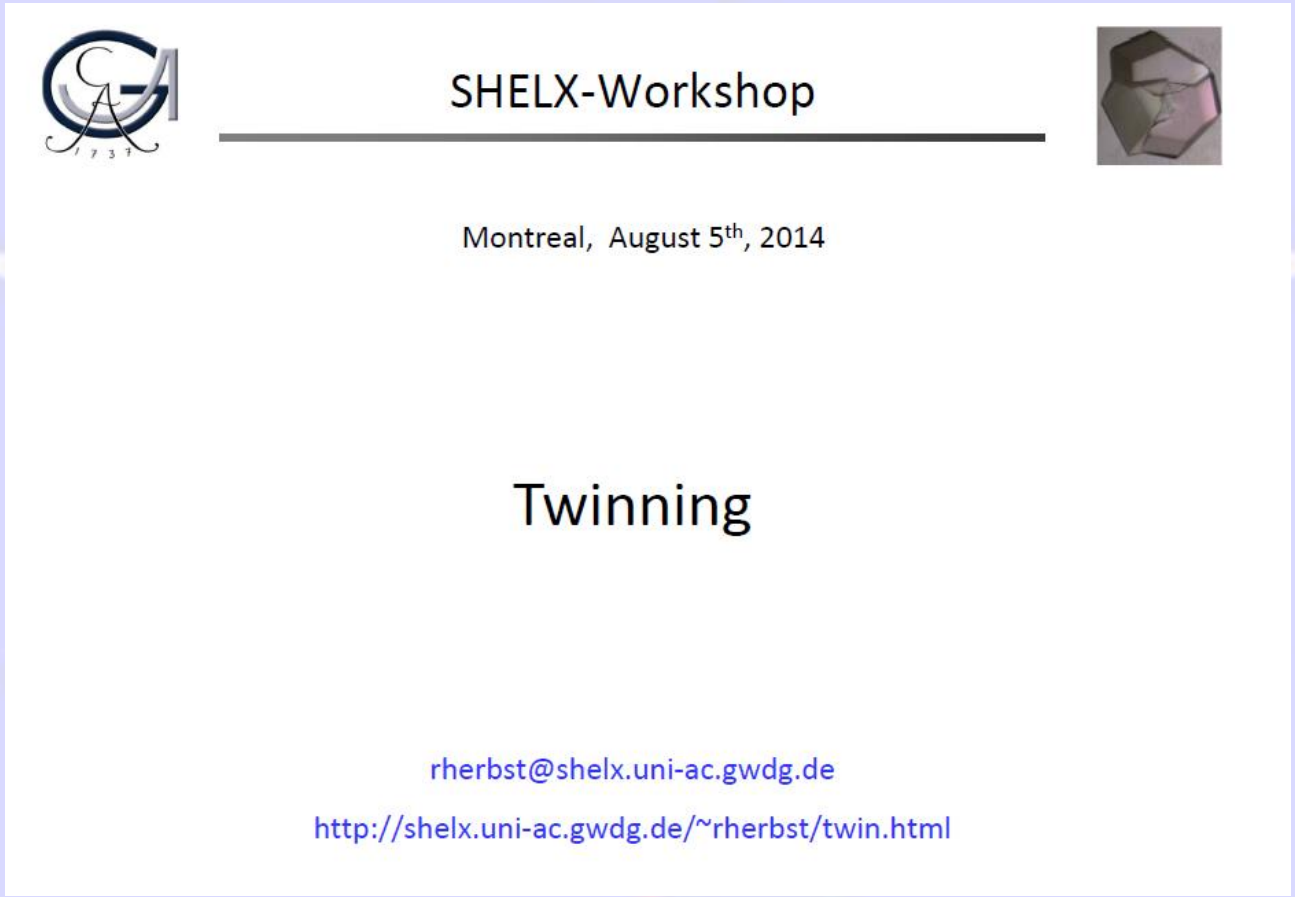
Cracked crystal. Random angle between orientations.

Growth of thin plate on a thin plate. Random angle between orientations.

Two different crystals stuck to each other. Different cells and space groups. Different compounds.

We can use the same software packages to clean up the mess.

Thanks to Regine Herbst-Irmer and . . .



SHELX-Workshop

Montreal, August 5th, 2014

Twinning

rherbst@shelx.uni-ac.gwdg.de

http://shelx.uni-ac.gwdg.de/~rherbst/twin.html

. . . Ton Spek for teaching me about twinning.

The PLATON/TwinRotMat Tool for Twinning Detection

Ton Spek
National Single Crystal Service Facility,
Utrecht University,
The Netherlands.

Delft, 29-Sept-2008

Thank You