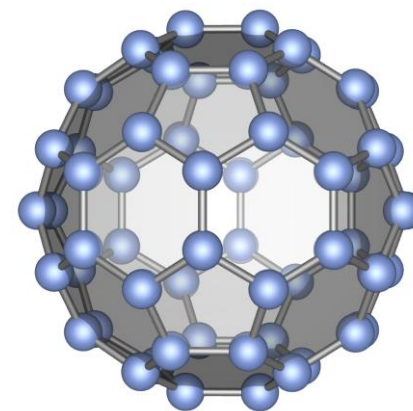
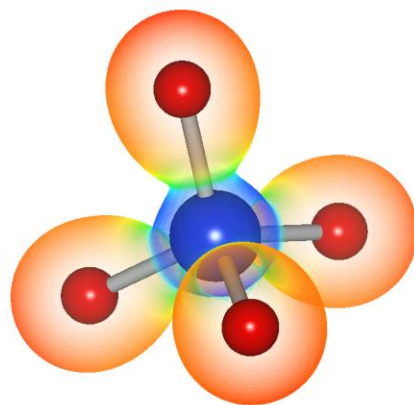
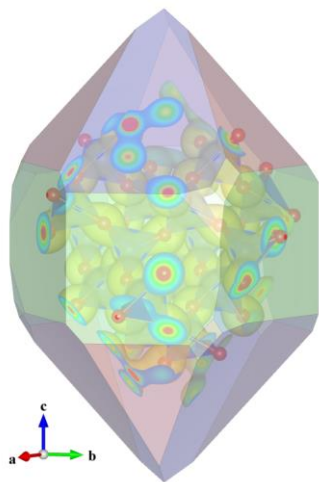


Symmetry, topology, and visualization of crystal structures

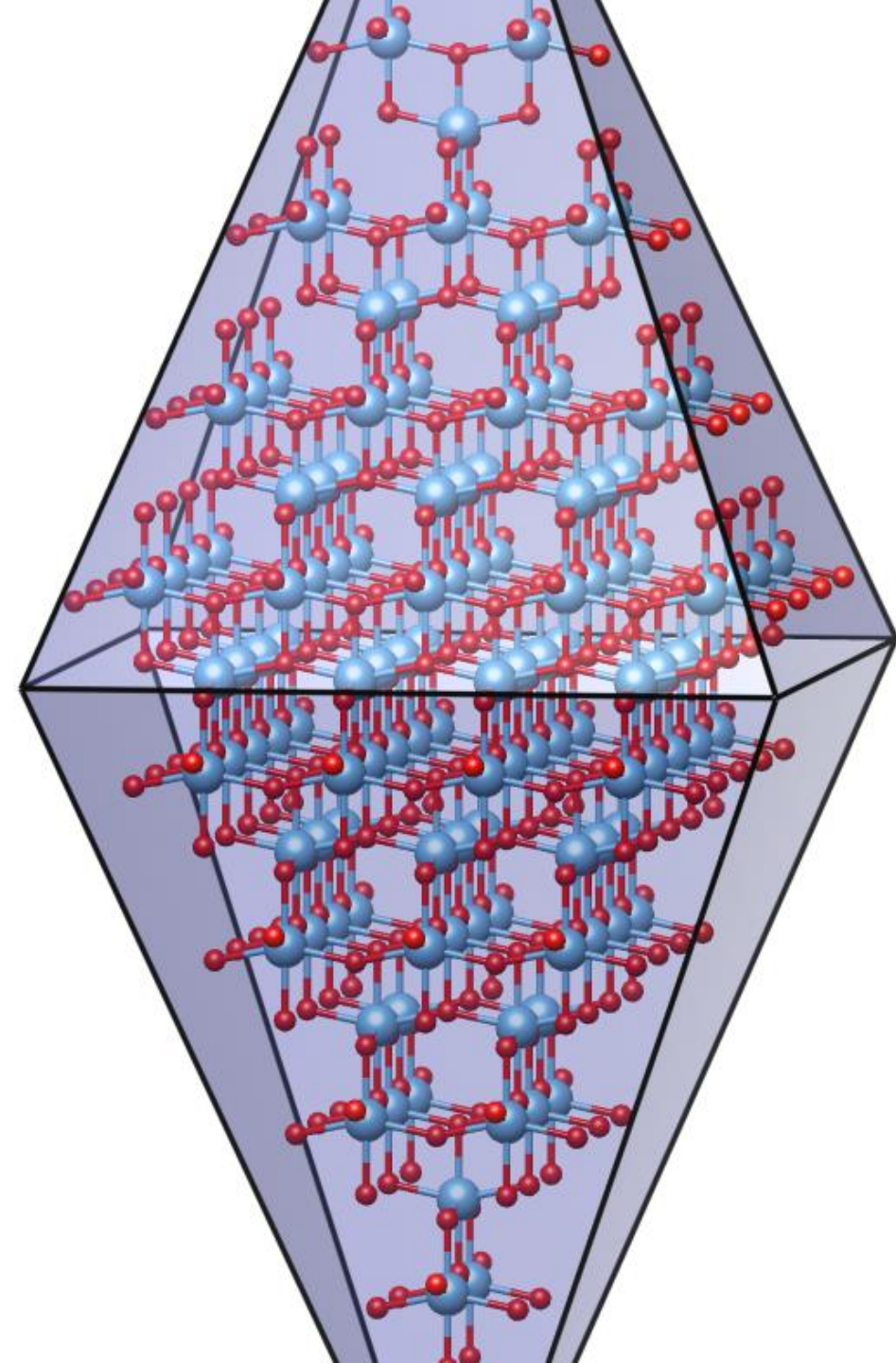


Koichi Momma

(National Museum of Nature and Science)

門馬綱一 (国立科学博物館)

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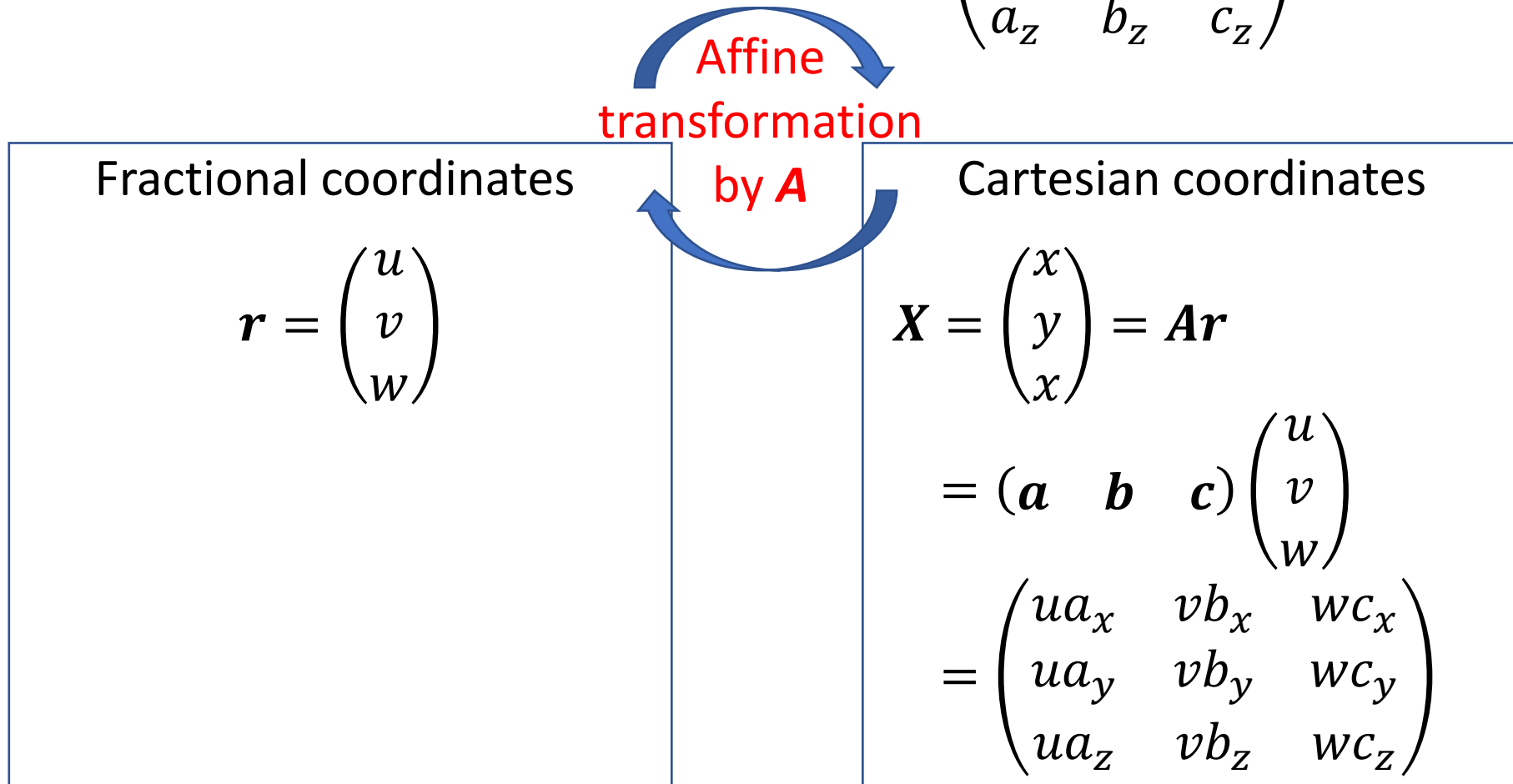
Contents

- Basic linear algebra in crystallography
- Conversions and comparison of structures using VESTA
- Command line interface of VESTA
- Practices

Unit cell

Representation of a unit cell $\mathbf{A} = (\mathbf{a} \quad \mathbf{b} \quad \mathbf{c})$

$$= \begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}$$



Metric matrix

Choice of **A** is arbitrary

VESTA adopts the following convention

$$\mathbf{A} = \begin{pmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{pmatrix}$$

Alternatively, you can choose

$$\mathbf{A} = \begin{pmatrix} a_x & 0 & 0 \\ a_y & b_y & 0 \\ a_z & b_z & c_z \end{pmatrix}$$

or any other orientation

$$\begin{aligned} \mathbf{G} &= \mathbf{A}^T \cdot \mathbf{A} \\ &= \begin{pmatrix} a^2 & a.b & a.c \\ a.b & b^2 & b.c \\ a.c & b.c & c^2 \end{pmatrix} \end{aligned}$$

G does not depend on choice of **A**.
It is unique for a given set of unit cell parameters.

Unit cell volume: $V^2 = \det(\mathbf{G})$

Reciprocal lattice and metric matrix of reciprocal lattice

Reciprocal lattice

$$\begin{aligned} \mathbf{A}^* &= \mathbf{A}^{-1} = \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} \\ &= \begin{pmatrix} a_x^* & a_y^* & a_z^* \\ b_x^* & b_y^* & b_z^* \\ c_x^* & c_y^* & c_z^* \end{pmatrix} \end{aligned}$$

Metric matrix

$$\begin{aligned} \mathbf{G}^* &= \mathbf{G}^{-1} = (\mathbf{A}^T \cdot \mathbf{A})^{-1} \\ &= (\mathbf{A}^* \cdot \mathbf{A}^{*T}) \\ &= \begin{pmatrix} \mathbf{a}^{*2} & \mathbf{a}^* \cdot \mathbf{b}^* & \mathbf{a}^* \cdot \mathbf{c}^* \\ \mathbf{a}^* \cdot \mathbf{b}^* & \mathbf{b}^{*2} & \mathbf{b}^* \cdot \mathbf{c}^* \\ \mathbf{a}^* \cdot \mathbf{c}^* & \mathbf{b}^* \cdot \mathbf{c}^* & \mathbf{c}^{*2} \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \mathbf{A}^* \mathbf{A} &= \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} (\mathbf{a} \quad \mathbf{b} \quad \mathbf{c}) \\ &= \begin{pmatrix} \mathbf{a}^* \cdot \mathbf{a} & \mathbf{a}^* \cdot \mathbf{b} & \mathbf{a}^* \cdot \mathbf{c} \\ \mathbf{b}^* \cdot \mathbf{a} & \mathbf{b}^* \cdot \mathbf{b} & \mathbf{b}^* \cdot \mathbf{c} \\ \mathbf{c}^* \cdot \mathbf{a} & \mathbf{c}^* \cdot \mathbf{b} & \mathbf{c}^* \cdot \mathbf{c} \end{pmatrix} = \mathbf{I} \end{aligned}$$

$$\mathbf{G}^* \mathbf{G} = \mathbf{G} \mathbf{G}^* = \mathbf{I}$$

Reciprocal lattice vectors

Reciprocal lattice vector

$$\mathbf{h} = (h \quad k \quad l)$$

Cartesian coordinates

$$\begin{aligned} \mathbf{X}^* &= (x \quad y \quad z) = \mathbf{h} \mathbf{A}^* \\ &= (h \quad k \quad l) \begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} \end{aligned}$$

- Normal vector of lattice plane $(h \ k \ l)$
- Length of the reciprocal lattice vector corresponds to $1/d$, where d is inter-planar spacing of $(h \ k \ l)$

Scalar products: $\mathbf{X}^* \mathbf{X} = \mathbf{h} \mathbf{A}^* \mathbf{A} \mathbf{r} = (h \quad k \quad l) \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \mathbf{h} \mathbf{r}$

$$\frac{1}{d^2} = \mathbf{d}^{*2} = \mathbf{X}^* (\mathbf{X}^*)^T = \mathbf{h} \mathbf{A}^* (\mathbf{h} \mathbf{A}^*)^T = \mathbf{h} \mathbf{A}^* \mathbf{A}^{*T} \mathbf{h}^T = (h \quad k \quad l) \mathbf{G}^* \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

Symmetry operations

Coordinates

$$\mathbf{X} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Symmetry operations

Mirror, inversion, rotation,
rotoinversion

translation

$$\mathbf{W} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix},$$

$$\mathbf{w} = \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix}$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix}$$

$$\mathbf{X}' = \mathbf{W}\mathbf{X} + \mathbf{w}$$

Symmetry operations

Coordinates

$$\mathbb{X} = \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

Symmetry operations

$$\mathbb{W} = \begin{pmatrix} \mathbf{W} & \mathbf{w} \\ \mathbf{o} & 1 \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} & w_x \\ W_{21} & W_{22} & W_{23} & w_y \\ W_{31} & W_{32} & W_{33} & w_z \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} & w_x \\ W_{21} & W_{22} & W_{23} & w_y \\ W_{31} & W_{32} & W_{33} & w_z \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

$$\mathbb{X}' = \mathbb{W}\mathbb{X}$$

By using additional row to make the matrix square, inverse operation can be easily computed by $\mathbb{W}^{-1}$.

Transformation of coordinate systems

$$\mathcal{P} = \begin{pmatrix} \mathbf{P} & \mathbf{p} \\ \mathbf{o} & 1 \end{pmatrix}$$

$$\begin{aligned} \mathcal{Q} = \mathcal{P}^{-1} &= \begin{pmatrix} \mathbf{P} & \mathbf{p} \\ \mathbf{o} & 1 \end{pmatrix}^{-1} \\ &= \begin{pmatrix} \mathbf{P}^{-1} & -\mathbf{P}^{-1}\mathbf{p} \\ \mathbf{o} & 1 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \mathcal{Q} &= \begin{pmatrix} \mathbf{Q} & \mathbf{q} \\ \mathbf{o} & 1 \end{pmatrix} \\ &= \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{aligned}$$

3 × 3 rotation part

3 × 1 translation part

Basis vectors:

$$\mathbf{A}' = \mathbf{A}\mathbf{P}$$

Metric matrix:

$$\mathbf{G}' = \mathbf{P}^T \mathbf{G} \mathbf{P}$$

Metric matrix:

$$\mathbf{G}^{*'} = \mathbf{Q} \mathbf{G}^* \mathbf{Q}^T$$

Coordinates:

$$\mathbf{X}' = \mathbf{Q} \mathbf{X}$$

Miller indices:

$$\mathbf{h}' = \mathbf{h} \mathbf{P}$$

Symmetry operations: $\mathbf{W}' = \mathbf{Q} \mathbf{W} \mathbf{P}$

The same relation is also true when dimension > 3

Definition of a group

- Identity element

There exists an element e in G such that,
 $e \bullet a = a \bullet e = a$ for any element a in G .

- Inverse element

For each a in G , there exists an inverse element a^{-1} in G , such that
 $a \bullet a^{-1} = a^{-1} \bullet a = e$

- Associative

For all a, b and c in G , $(a \bullet b) \bullet c = a \bullet (b \bullet c)$.

- Closed

For all a, b in G , $a \bullet b$, is also in G .

Generators of symmetry operations

Generators of the icosahedral space group $Fm\overline{3}5$ ($m\overline{3}5^2$)

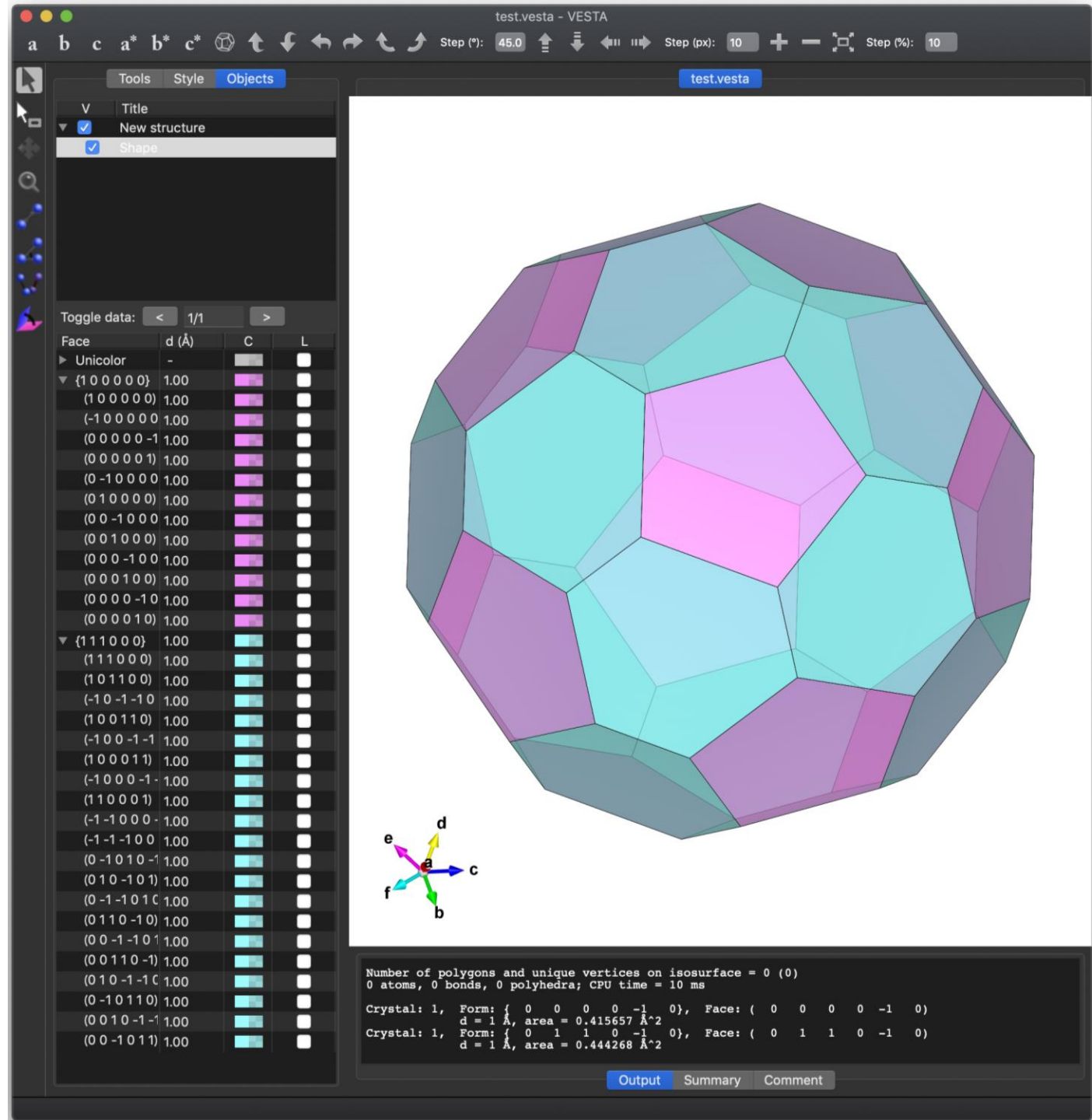
$$R_{51} \equiv x, w, y, z, u, v$$

$$R_{31} \equiv y, z, x, w, -u, -v$$

$$R_{21} \equiv -x, -y, -w, -v, -u, -z$$

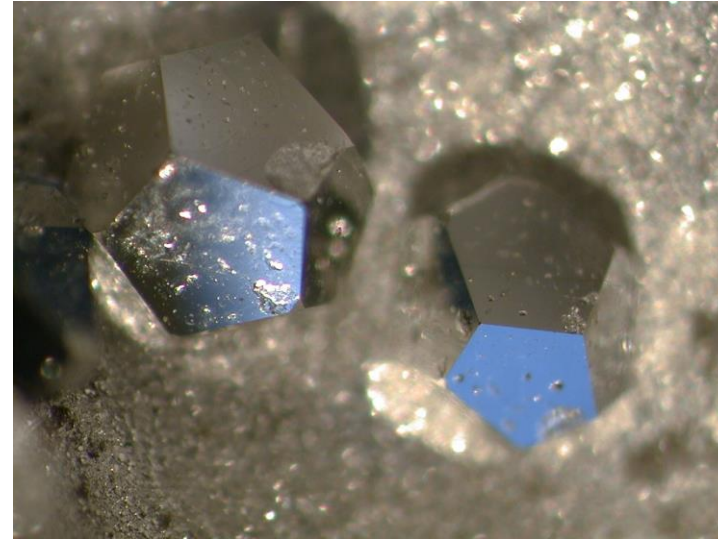
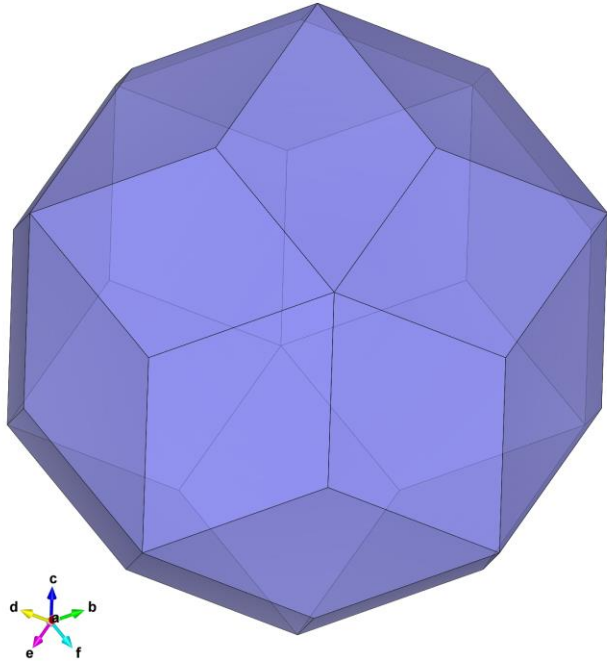
$$I \equiv -x, -y, -z, -u, -v, -w$$

$$(t \equiv 1/2, 1/2, 0, 0, 0, 0)$$



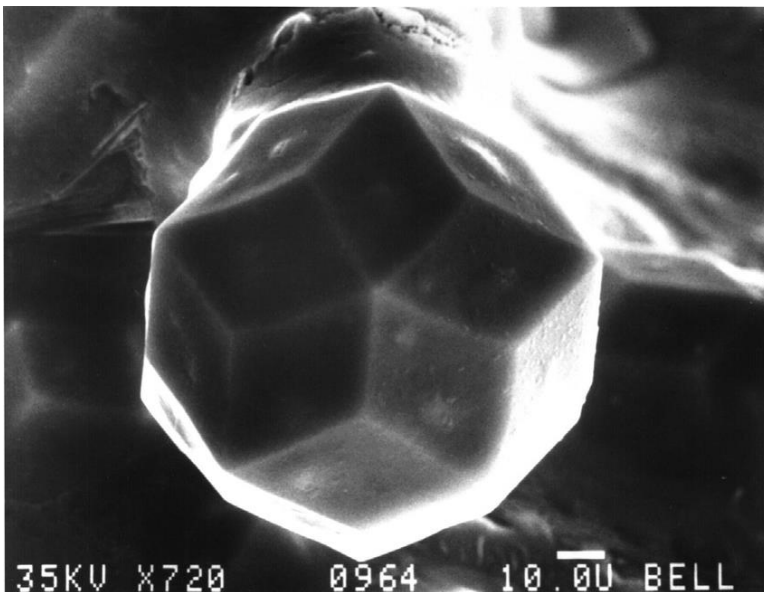
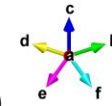
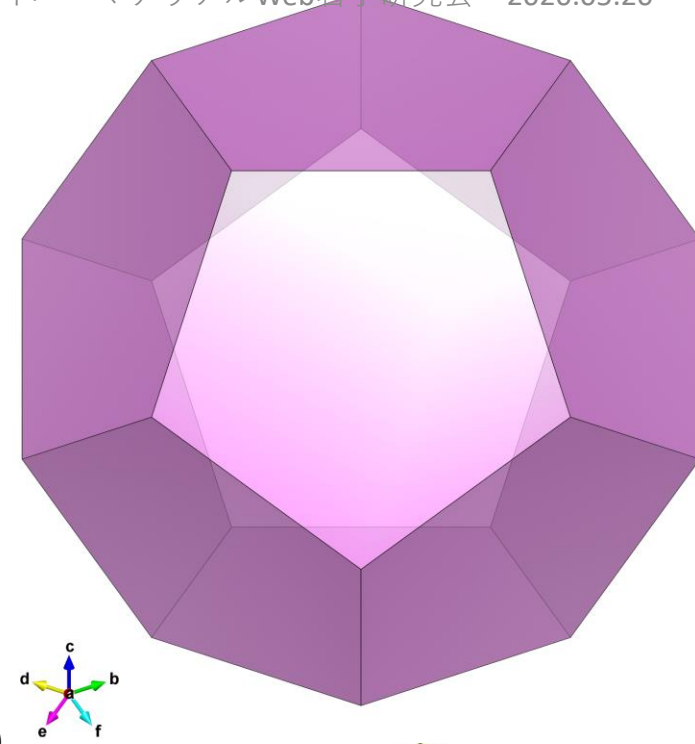
Visualization of quasicrystal morphology

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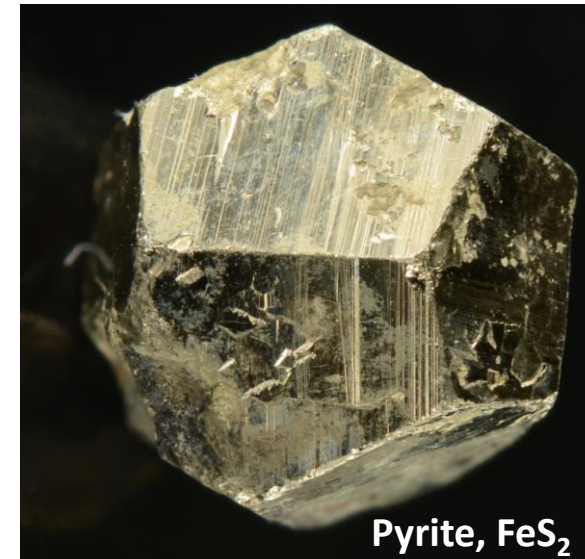


Zn-Mg-Dy decagonal phase

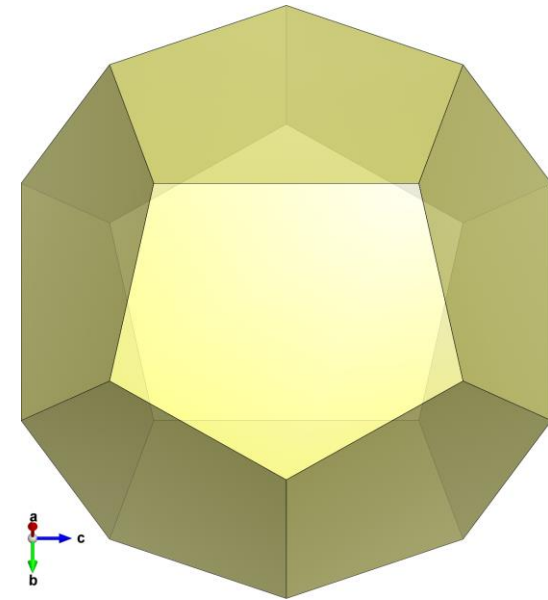
(撮影: 蔡安邦教授)



Rhombic triacontahedral morphology
in Al-Li-Cu alloy
(Kortan et al., 1989)

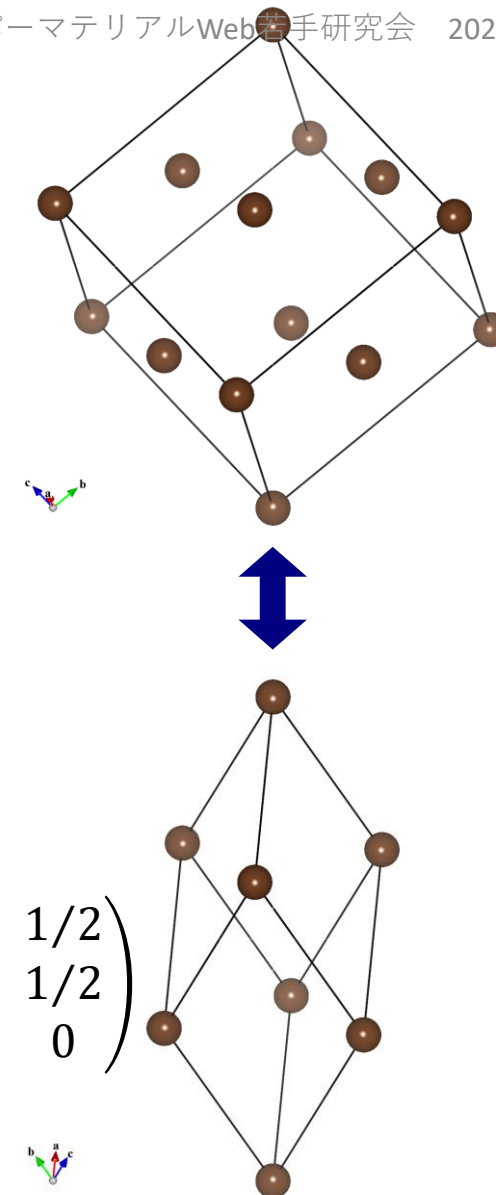
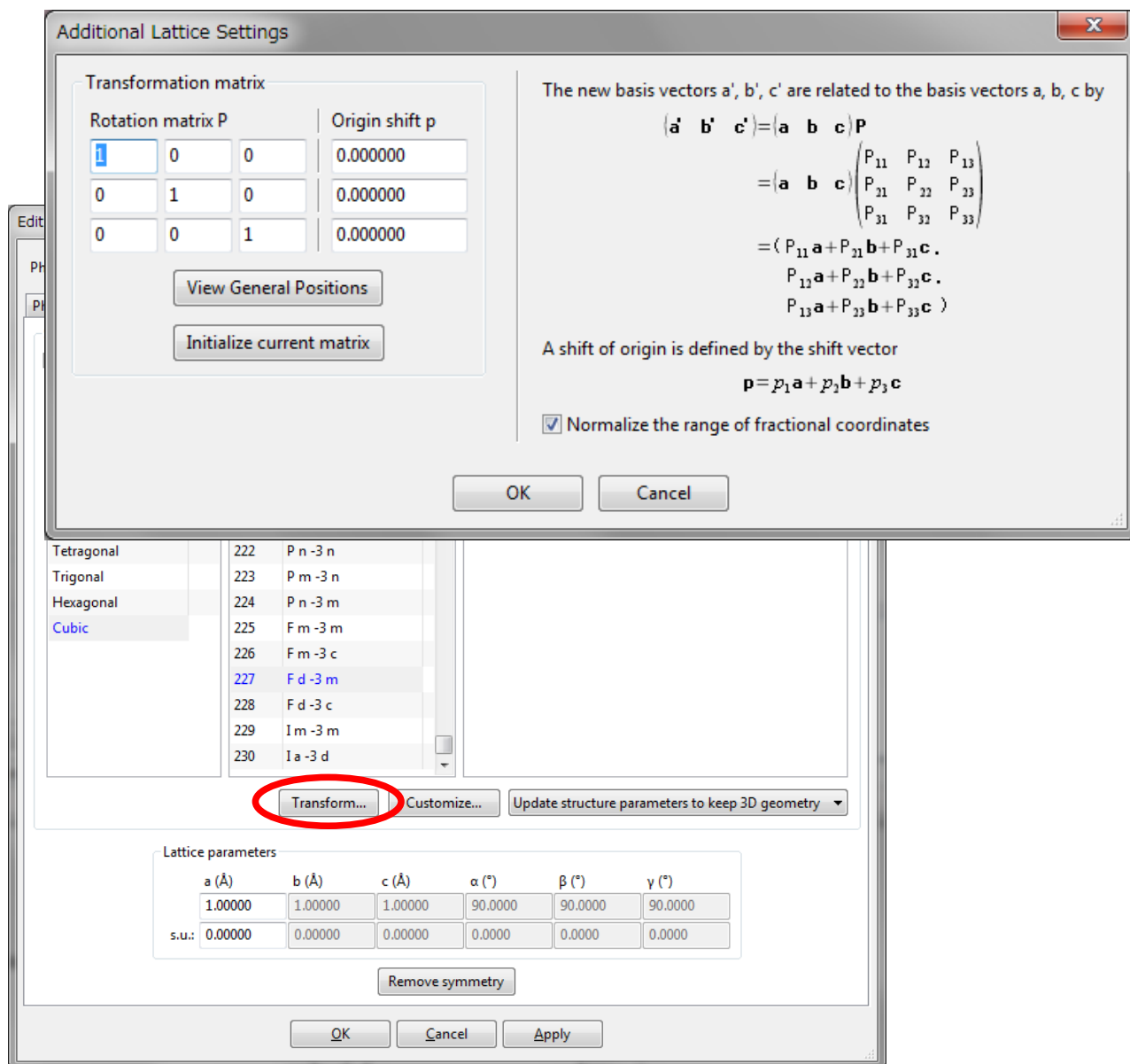


Pyrite, FeS₂



Transformation of coordinate systems

- Edit → Edit Data → Unit cell → Transform



$$F \rightarrow P$$

$$\begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix}$$

$$P \rightarrow F$$

$$\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

Transformation of coordinate systems

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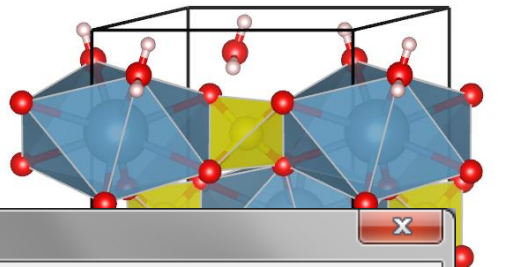


Diagram illustrating the transformation of coordinate systems. A 3D model of a crystal structure is shown, with atoms represented by red spheres and polyhedra in blue and yellow. Arrows indicate the transformation process from the initial structure to the transformed structure.

Edit Data - CaTiO3.cif

Phase: 1 Ca O3 Ti

Phase Unit cell Structure parameters Volumetric data Crystal shape

Atomic displacement parameter Anisotropic: U Isotropic: B

No.: 2/4 Symbol... Ca Label: Ca1 Charge: 2

x: 0.006480 y: 0.035600 z: 0.250000 Occ.: 1

s.u.(x): 0.000080 s.u.(y): 0.000100 s.u.(z): 0.000000 B: 0.642182

U11: 0.008200 U22: 0.008300 U33: 0.007900

U12: 0.001600 U13: 0.000000 U23: 0.000000

No.	Atom	Label	x	y	z	Occ.	B
1	Ti	Ti1	0.000000	0.500000	0.000000	1	0.410576
2	Ca	Ca1	0.006480	0.035600	0.250000	1	0.642182
3	O	O1	0.571100	-0.016100	0.250000	1	0.560594
4	O	O2	0.289700	0.288800	0.037300	1	0.579017

New Delete Clear

Import...

Link

Remove duplicate atoms

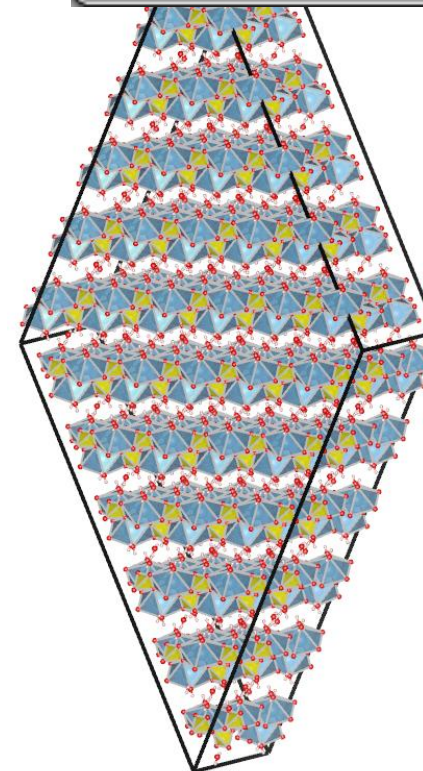
OK Cancel Apply

Additional lattice point(s) are included in the new unit...

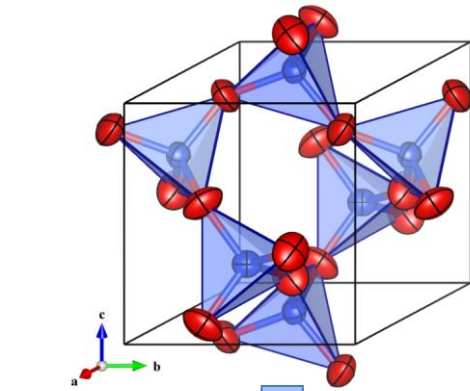
How to convert the structure?

- ☒ Add new equivalent positions to a list of symmetry operations
- ☐ Search atoms in the new unit-cell and add them as new sites
- ☐ Do nothing

OK



Conversion of a structure to its subgroup / supergroup



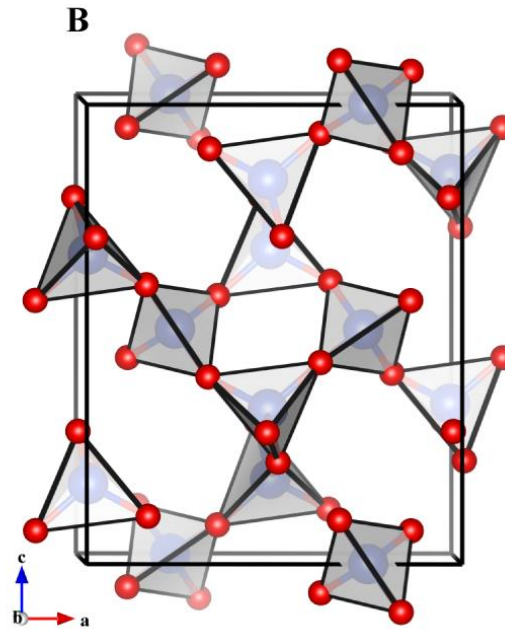
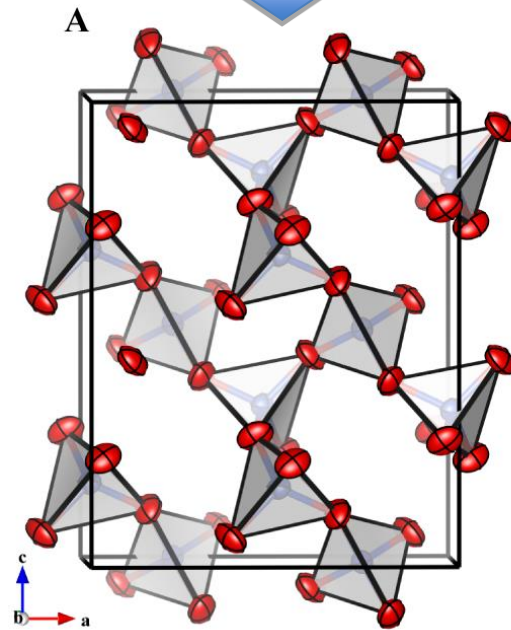
$$P3_121 \rightarrow C2 \quad C2 \rightarrow C2 \text{ with } c'=2c$$

$$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Transformation matrix

Translation of the origin

New basis vectors a' , b' , c' , specified by lattice vectors $[u \ v \ w]$ (column vector) using basis vectors of the current setting.



A: A monoclinic setting of quartz unit cell with $a'=2a+b$, $b'=b$, and $c'=2c$. B: Unit cell of a silica polymorph moganite.

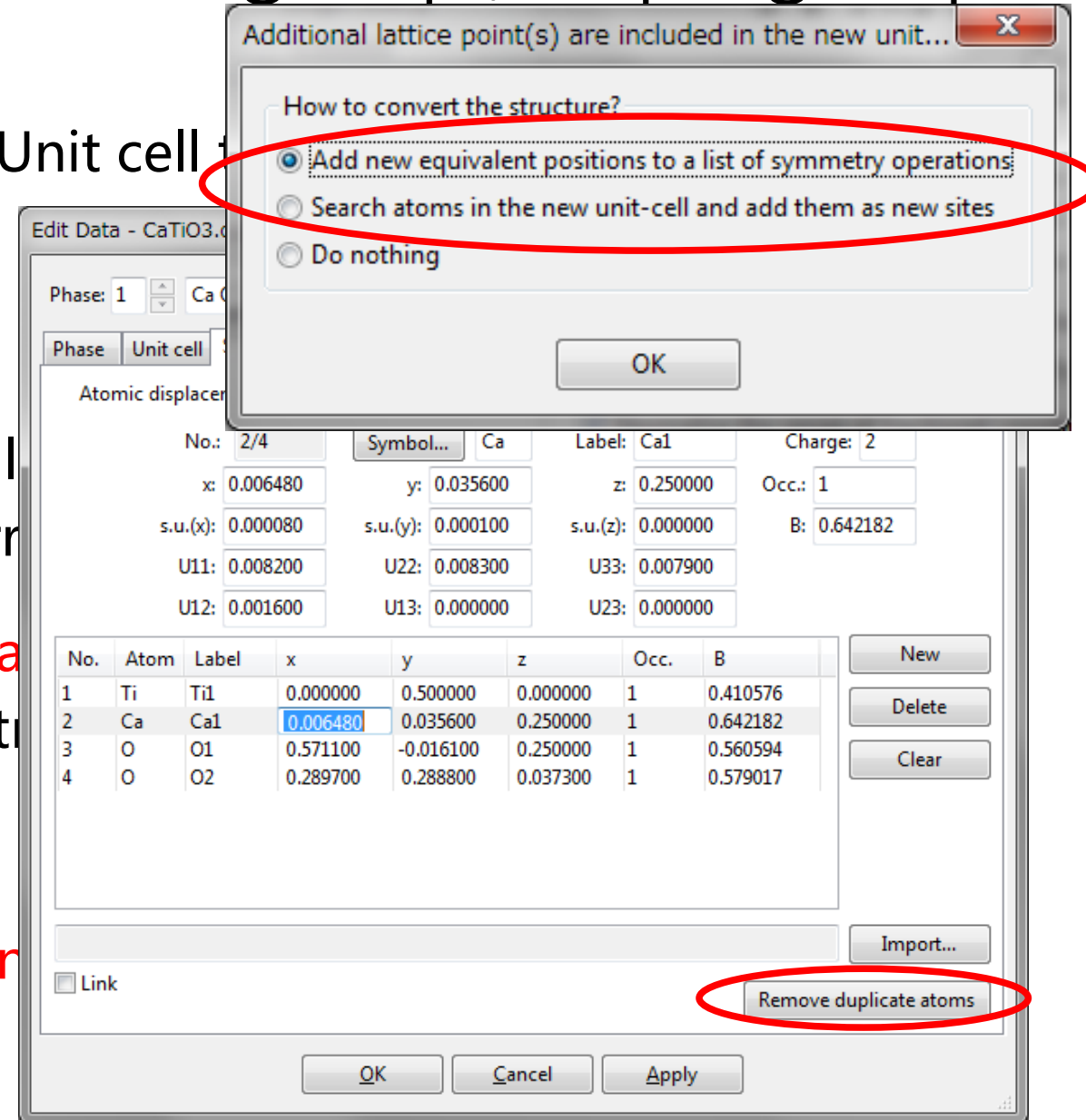
Practice 1 – 3

Conversion of a structure to its subgroup / supergroup

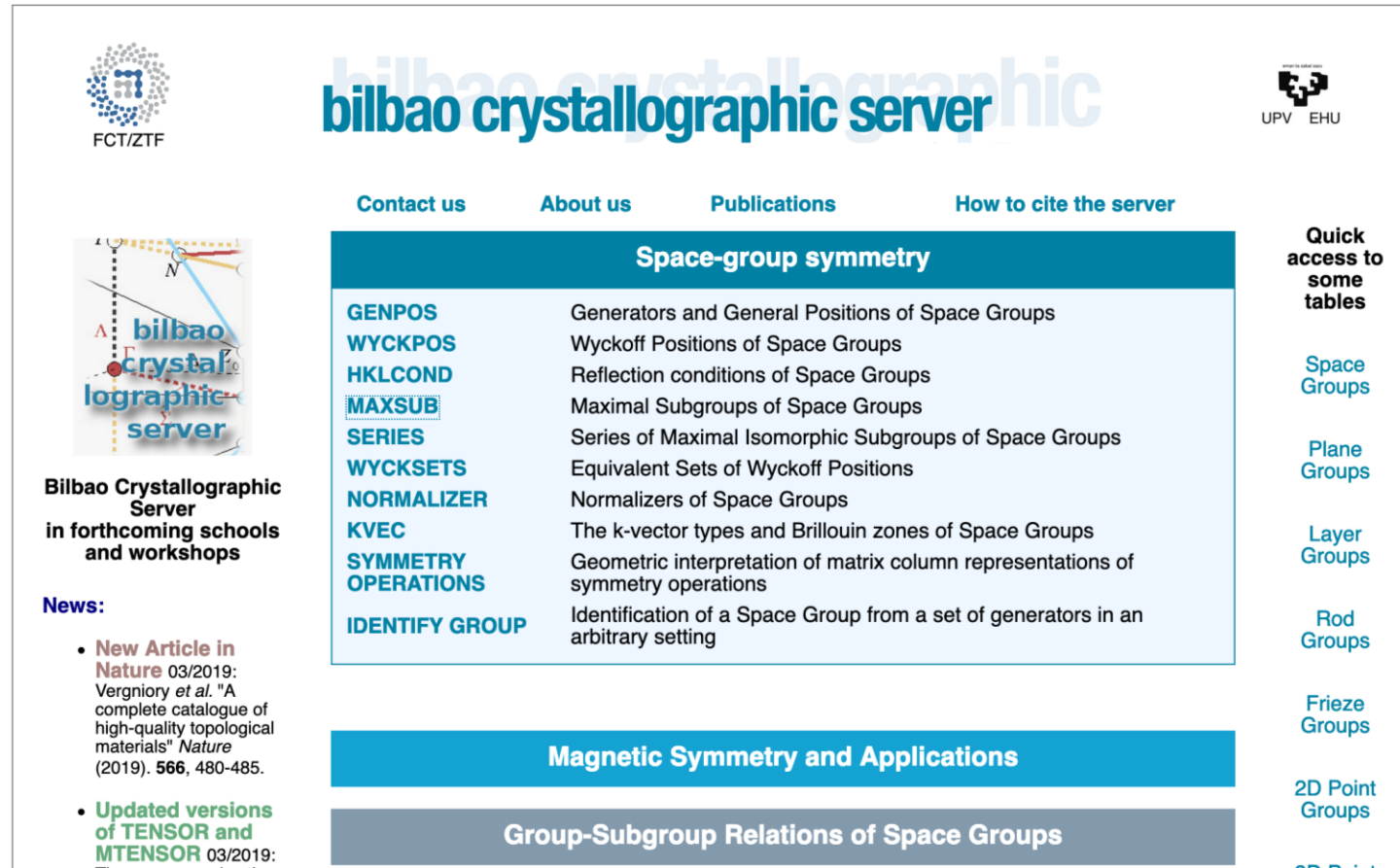
- Press "Remove Symmetry" button in the Unit cell tab in Edit Data dialog box (When symmetry lowers)
- Set a transformation matrix.
- Automatically search and add additional lattice points or additional sites if necessary. (The structure should look correct at this step)
- **Press the "Remove Symmetry" button again.** (This operation will reset the transformation matrix to the identity matrix.)
- Set a new space group.
- **Use the "Remove duplicate atoms" button.** (Merge closely adjacent atoms into single site)

Conversion of a structure to its subgroup / supergroup

- Press "Remove Symmetry" button in the Unit cell tab (When symmetry lowers)
- Set a transformation matrix.
- Automatically search and add additional lattice points if necessary. (The structure should look correct)
- Press the "Remove Symmetry" button again to reset the transformation matrix to the identity matrix
- Set a new space group.
- Use the "Remove duplicate atoms" button (to remove atoms on the same site)



Conversion of a structure to its subgroup / supergroup



The screenshot shows the Bilbao Crystallographic Server homepage. At the top, there are logos for FCT/ZTF, the server name 'bilbao crystallographic server', and UPV/EHU. Navigation links include 'Contact us', 'About us', 'Publications', and 'How to cite the server'. A central table lists tools under the heading 'Space-group symmetry'. To the right, a sidebar provides 'Quick access to some tables' with links for Space Groups, Plane Groups, Layer Groups, Rod Groups, Frieze Groups, and 2D Point Groups. On the left, there is a section for 'Bilbao Crystallographic Server in forthcoming schools and workshops' and a 'News' section with two bullet points about recent publications in Nature.

bilbao crystallographic server

FCT/ZTF UPV/EHU

Contact us About us Publications How to cite the server

Space-group symmetry

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Quick access to some tables

- Space Groups
- Plane Groups
- Layer Groups
- Rod Groups
- Frieze Groups
- 2D Point Groups

Bilbao Crystallographic Server in forthcoming schools and workshops

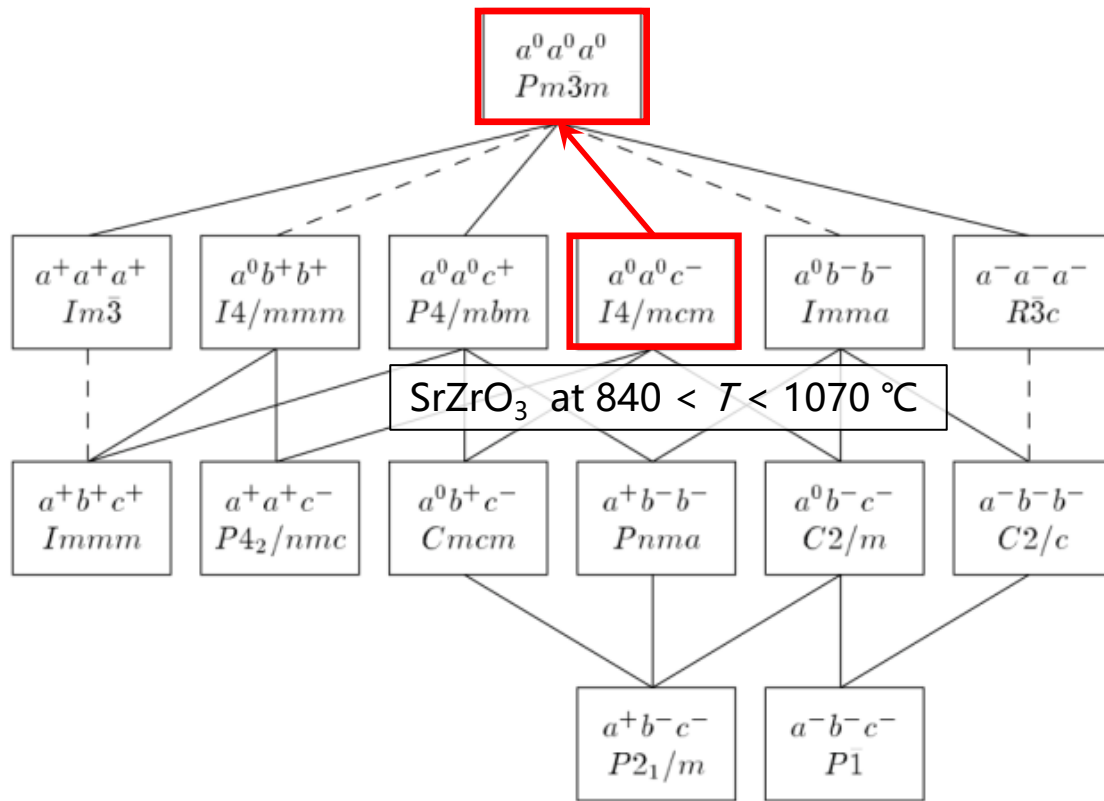
News:

- **New Article in Nature** 03/2019: Vergniory *et al.* "A complete catalogue of high-quality topological materials" *Nature* (2019). **566**, 480-485.
- **Updated versions of TENSOR and MTENSOR** 03/2019:

Bilbao crystallographic server (<http://www.cryst.ehu.es/>)

- Space-group symmetry -> MAXSUB
- Group-Subgroup Relations of Space Groups -> MINSUP

Conversion of a structure to its subgroup / supergroup



A schematic diagram indicating the group–subgroup relationships among the 15 space groups associated with octahedral tilting in perovskites (Howard et al., 2000).

Even with MINSUP,
transformation matrix from
supergroup $\rightarrow$ subgroup is shown.
For inverse conversion, inversion
matrix needs to be calculated

$$I4/mcm \leftarrow P4/mmm \quad P4/mmm \leftarrow Pm3m$$

$$\begin{pmatrix} 1 & 1 & 0 & 1/2 \\ -1 & 1 & 0 & 1/2 \\ 0 & 0 & 2 & 1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Inversion matrix ($I4/mcm \rightarrow Pm3m$)

$$\begin{pmatrix} 1/2 & -1/2 & 0 & 0 \\ 1/2 & 1/2 & 0 & -1/2 \\ 0 & 0 & 1/2 & -1/4 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Practice 4

Conversion of a structure to its supergroup without calculating inverse matrix

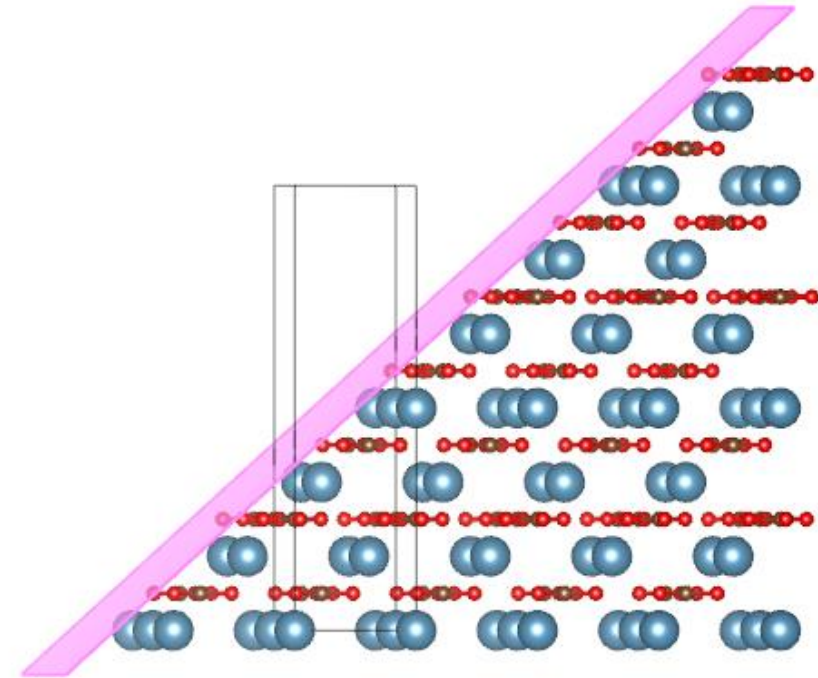
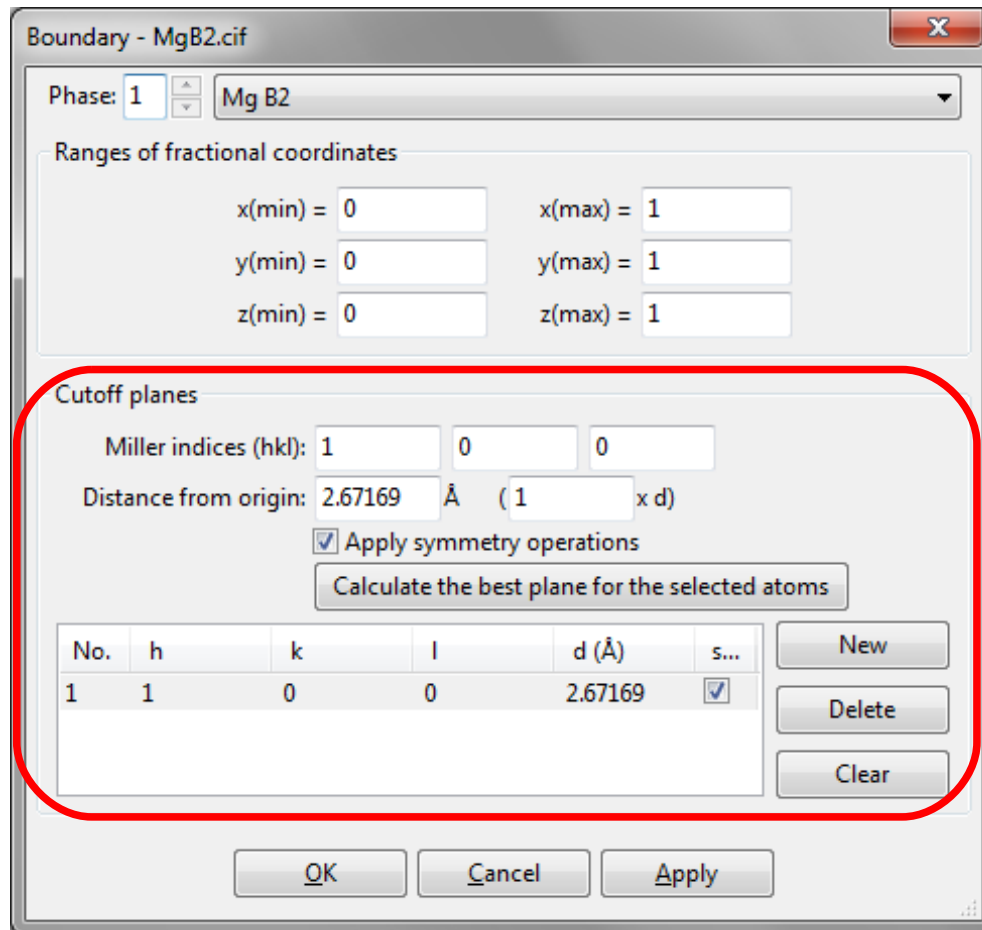
- In the “Edit Data” dialog box, **change an option to the “Keep structure parameters unchanged” mode**. Then input a transformation matrix from the desired **supergroup to the current space group**.

$$\begin{pmatrix} 1 & 1 & 0 & 1/2 \\ -1 & 1 & 0 & 1/2 \\ 0 & 0 & 2 & 1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The result will be the same as
“transformation from the supergroup
Pm3m to *I4/mcm*” by this matrix

- Revert to the “Update structure parameters to keep 3D geometry” mode.
- Open the Transform dialog again and revert the matrix to the identity matrix.
(**DO NOT use the Initialize button**. Input manually.)
- Change the space group to the supergroup.
- Use the “Remove duplicate atoms” if necessary.

Cut a structure by lattice planes



Practice 5

Command line interface of VESTA

Commands that work without GUI

- i *file* Read a file without visualization
- save *file* Save data to *file*.
parameters: *format=rietan; option=cartesian,pcell,reduced,as_displayed*
- list bond Output information of unique bonds in the text area
- list angle Output information of unique bond angles in the text area
- list poly Output information of unique polyhedra in the text area
- merge_split_site *dmin=x* Perform "Remove duplicate atoms"
- calcf out=*file* Calculate structure factors and output to *file*

parameters: *source=n lambda=x resolution=x anomalous=n*

source: 0: X-ray (default); 1: Neutron

lambda: wave length of the source in angstrom

resolution: minimum d-spacing of hkl in angstrom

(Blue letters are optional parameters)

Command line interface of VESTA

Commands that work without (continued)

-rotate_x <i>angle</i>	Rotate 3D graphics around the <i>x</i> -axis
-rotate_y <i>angle</i>	Rotate 3D graphics around the <i>y</i> -axis
-rotate_z <i>angle</i>	Rotate 3D graphics around the <i>z</i> -axis

Commands that can be used when GUI is executed

-open <i>file</i>	Read a <i>file</i> and visualize
-reopen <i>file</i>	Reload data from a <i>file</i> and update 3D graphics
-close <i>file</i>	Close a tab showing the <i>file</i> . Close currently selected tab if no file specified.
-export_img <i>scale=n file</i>	Export an image to <i>file</i> .
-flush	Update screen after some operation, e.g. rotating data

Command line interface of VESTA: Usage 1

Without GUI (combine with -nogui option)

- Windows & Linux

VESTA -nogui -i test.cif -o format=rietan test.ins

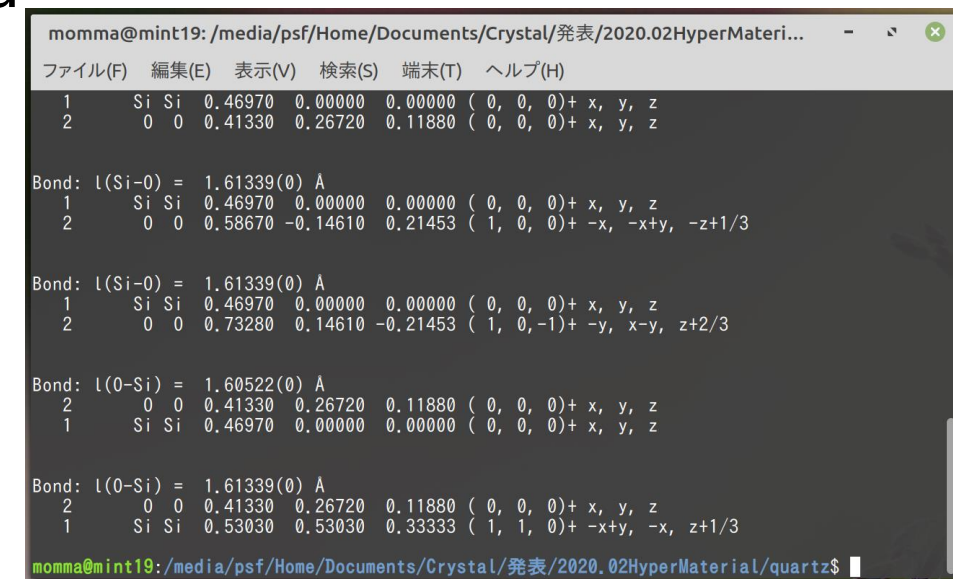
VESTA -nogui -i test.cif -o option=cartesian test.vasp

VESTA -nogui -i test.cif -list bond angle poly

(On windows, no texts will be output to the command prompt, so nothing happens on the last example)

- macOS

This mode does not currently work on macOS



```
momma@mint19: /media/psf/Home/Documents/Crystal/発表/2020.02HyperMateri...  
ファイル(F) 編集(E) 表示(V) 検索(S) 端末(T) ヘルプ(H)  
1      Si Si  0.46970  0.00000  0.00000 ( 0, 0, 0)+ x, y, z  
2      O  O  0.41330  0.26720  0.11880 ( 0, 0, 0)+ x, y, z  
  
Bond: l(Si-O) = 1.61339(0) Å  
1      Si Si  0.46970  0.00000  0.00000 ( 0, 0, 0)+ x, y, z  
2      O  O  0.58670 -0.14610  0.21453 ( 1, 0, 0)+ -x, -x+y, -z+1/3  
  
Bond: l(Si-O) = 1.61339(0) Å  
1      Si Si  0.46970  0.00000  0.00000 ( 0, 0, 0)+ x, y, z  
2      O  O  0.73280  0.14610 -0.21453 ( 1, 0,-1)+ -y, x-y, z+2/3  
  
Bond: l(O-Si) = 1.60522(0) Å  
2      O  O  0.41330  0.26720  0.11880 ( 0, 0, 0)+ x, y, z  
1      Si Si  0.46970  0.00000  0.00000 ( 0, 0, 0)+ x, y, z  
  
Bond: l(O-Si) = 1.61339(0) Å  
2      O  O  0.41330  0.26720  0.11880 ( 0, 0, 0)+ x, y, z  
1      Si Si  0.53030  0.53030  0.33333 ( 1, 1, 0)+ -x+y, -x, z+1/3  
momma@mint19: /media/psf/Home/Documents/Crystal/発表/2020.02HyperMaterial/quartz$
```

Command line interface of VESTA: Usage 2

With GUI (texts will be output to the text area of VESTA main window)

- Windows & Linux

VESTA -open test.cif

VESTA -list bond

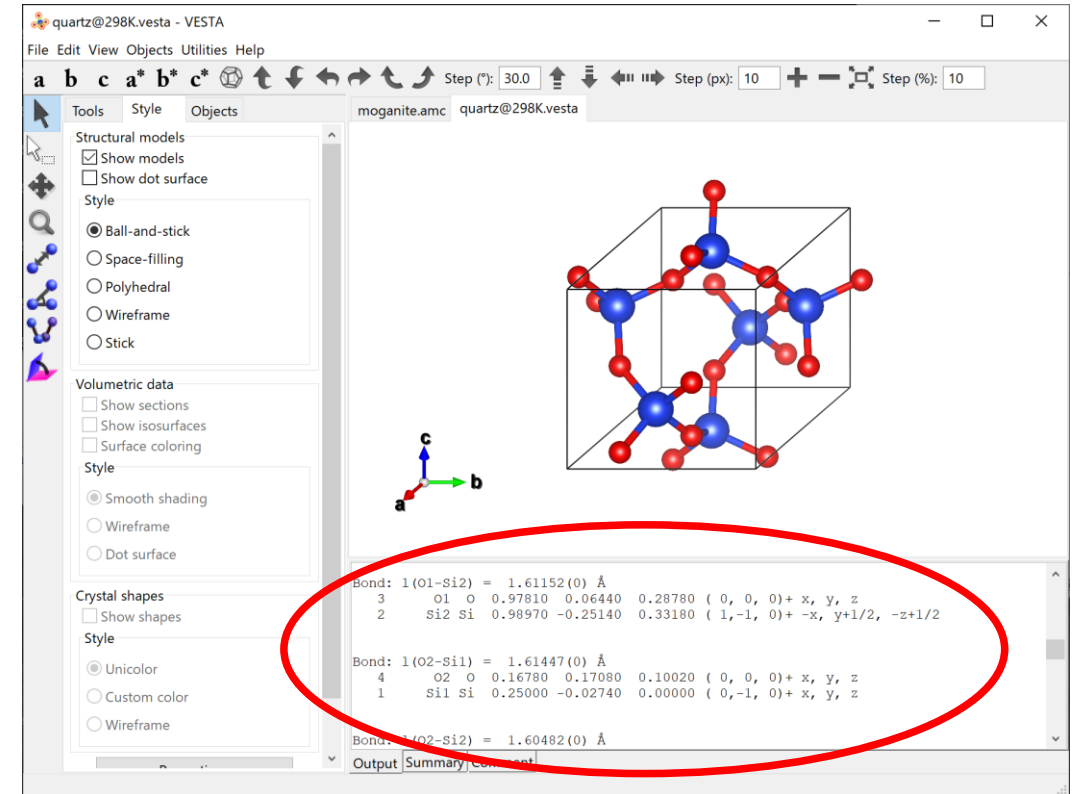
VESTA -export_img test.png

VESTA close

- macOS

open -n -a VESTA.app --args -list angle

open -n -a VESTA.app --args -save format=rietan test.ins



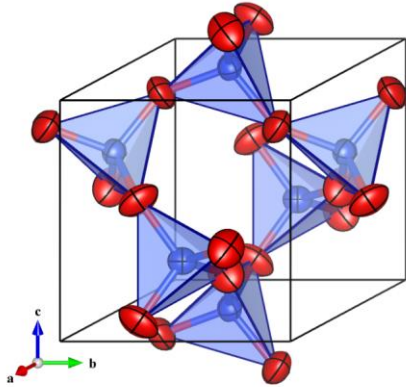
Practices

1. Comparison of two structures
2. Conversion of quartz structure
3. Align positions and orientations of data with different unit-cell settings
4. Conversion of SrZrO_3 from $I4/mcm$ to $Pm3m$
5. Align the (111) slice of Ir metal parallel to graphene
6. Find possible stacking sequences of polytypes

If you haven't installed VESTA on your PC yet,
please download the latest version from

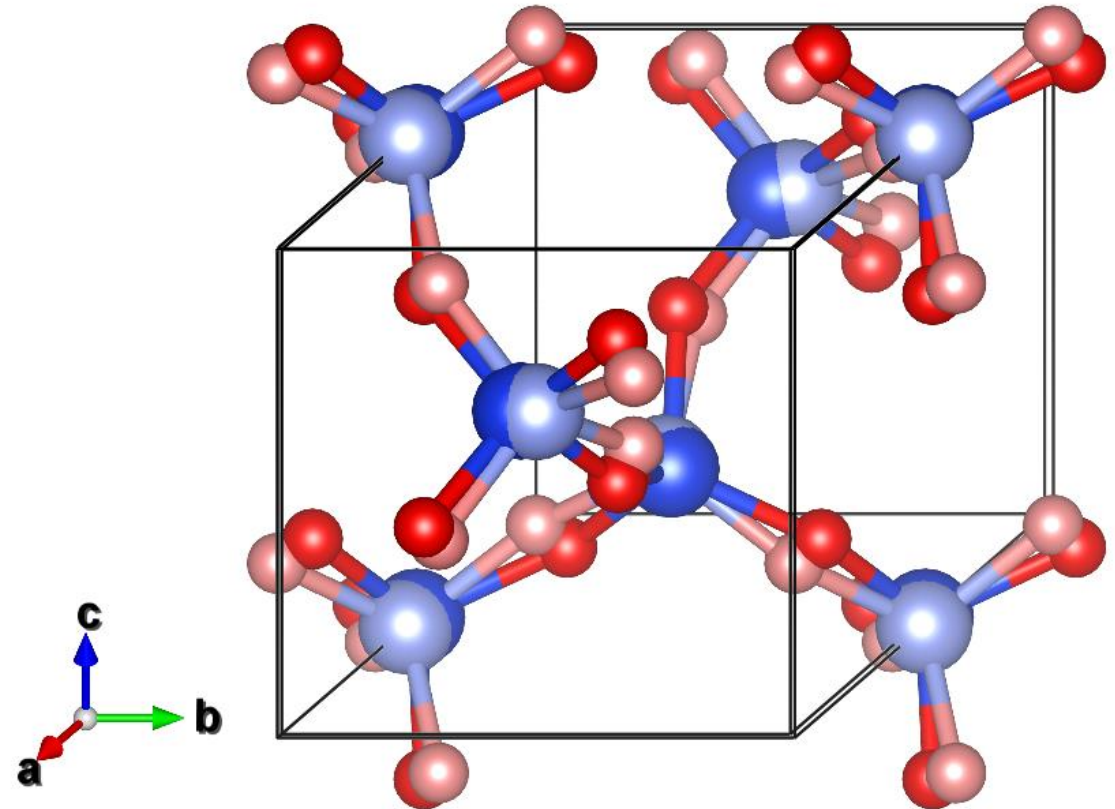
<http://jp-minerals.org/vesta/en/download.html>

Practice 1. Comparison of two structures

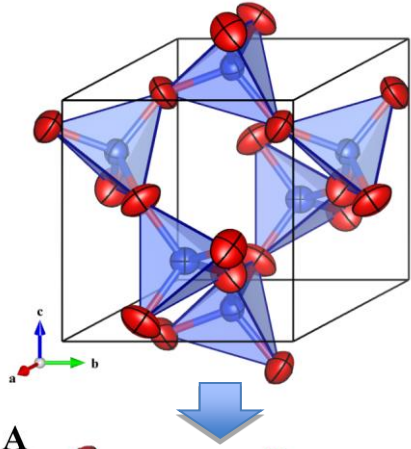


What to do: Align low-T and high-T data of quartz in the same window

1. Open quartz/quartz@298K.vesta
2. Import quartz/quartz@920K.amc
3. Set the origin of the low-T data to match with high-T data
(set 0,0,2/3 as the origin shift p of low-T data)

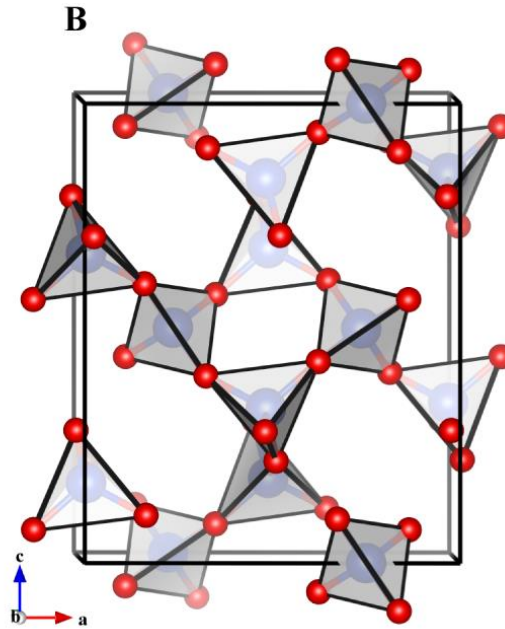
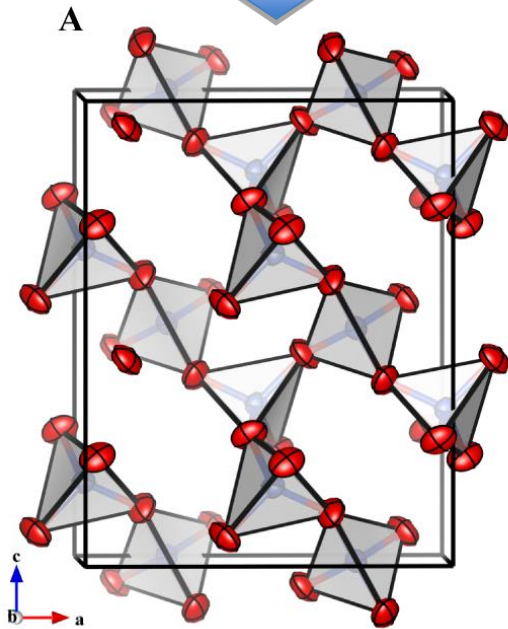


Practice 2. Conversion of quartz structure



$$P3_121 \rightarrow C2 \quad C2 \rightarrow C2 \text{ with } c'=2c$$

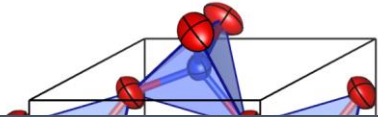
$$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1/3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



A: A monoclinic setting of quartz unit cell with $a'=2a+b$, $b'=b$, and $c'=2c$. B: Unit cell of a silica polymorph moganite.

1. Open quartz/quartz@298K.vesta
2. Remove symmetry
3. Set the above transformation matrix
4. Remove symmetry again (to reset the transformation matrix)
5. Set space group $C2$
6. Remove duplicate atoms
7. Compare with quartz/moganite.amc

Practice 2. Conversion of quartz structure



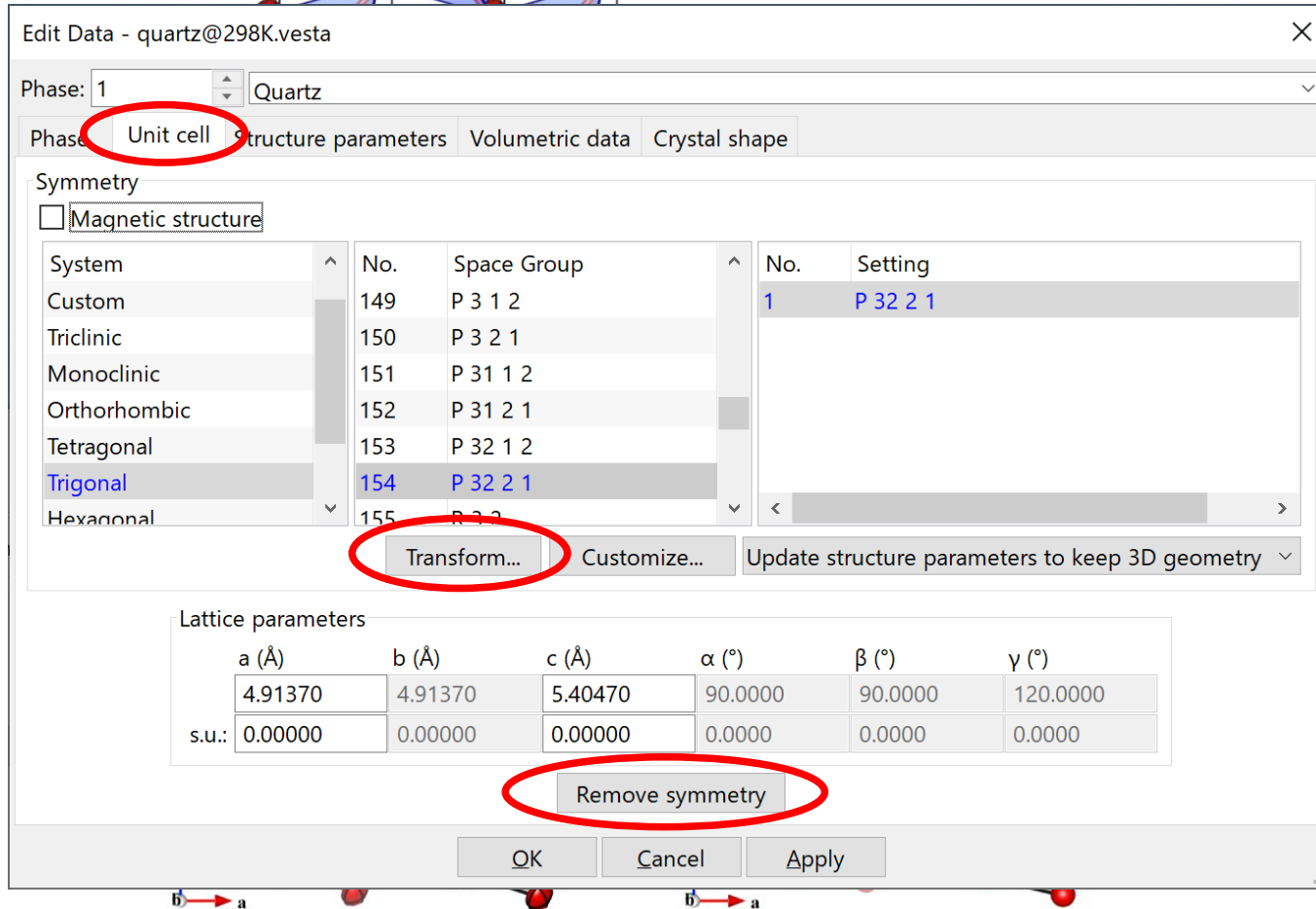
$$P3_121 \rightarrow C2$$

$$C2 \rightarrow C2$$

with $c'=2c$

Transformation matrix

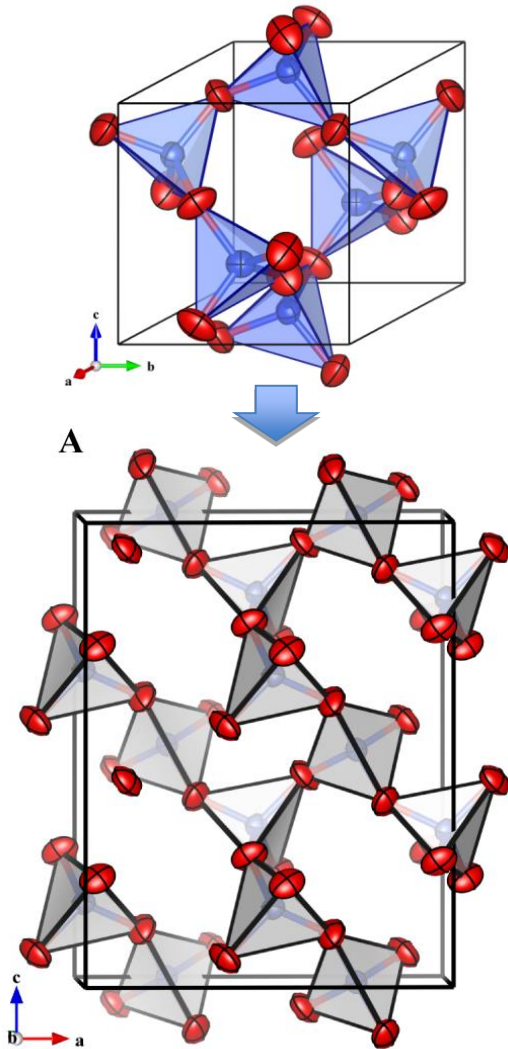
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 1/3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$



1. Open quartz/quartz@298K.vesta
2. Remove symmetry
3. Set the above transformation matrix
4. Remove symmetry again (to reset the transformation matrix)
5. Set space group $C2$
6. Remove duplicate atoms
7. Compare with quartz/moganite.amc

A: A monoclinic setting of quartz unit cell with $a'=2a+b$, $b'=b$, and $c'=2c$. B: Unit cell of a silica polymorph moganite.

Practice 3. Align positions and orientations of data with different unit-cell settings



1. Open the quartz data transformed to C2 cell in the practice 2.
2. Import the original quartz/quartz@298K.vesta
3. Align the 2nd data as

Phase: 2 Quartz trigonal

Phase Unit cell Structure parameters Volume data Crystal shape

$[210]_{\text{hex}} // [100]_{\text{mono}}$ $(001)_{\text{hex}} // (001)_{\text{mono}}$

No.	Title
1	Quartz monoclinic
2	Quartz trigonal

Positioning

Place (x,y,z) of this layer at (x,y,z) of layer 1

This layer	Layer 1
0 0 0.333333	0 0 0

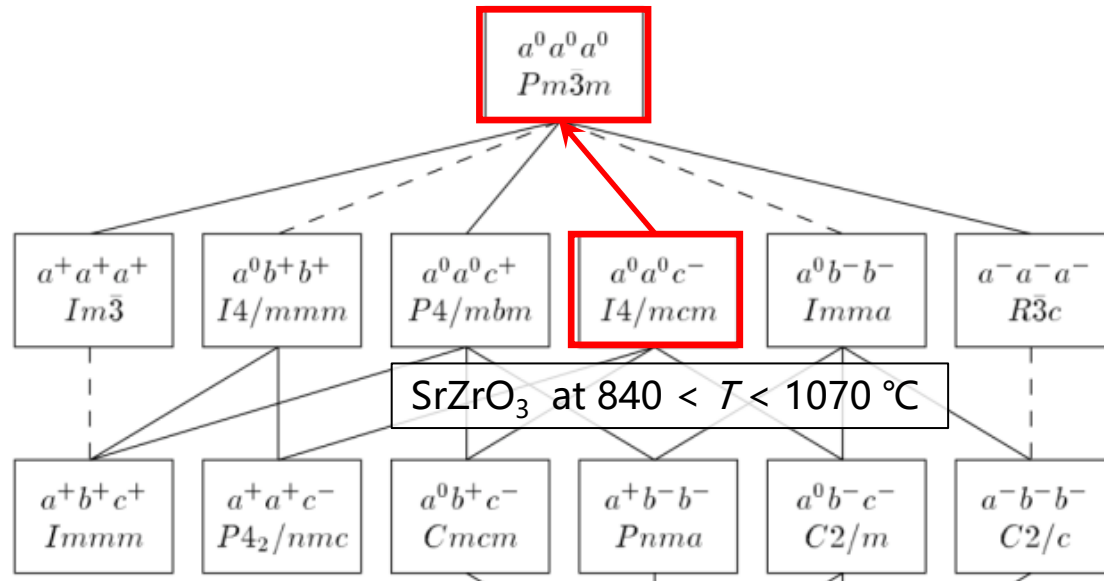
Orientation

Align orientation of this layer with respect to layer 1

This layer	Layer 1
[u v w] 2 1 0	[u v w] 1 0 0
(h k l) 0 0 1	(h k l) 0 0 1

OK Cancel Apply

Practice 4. Conversion of SrZrO_3 from $I4/mcm$ to $Pm3m$

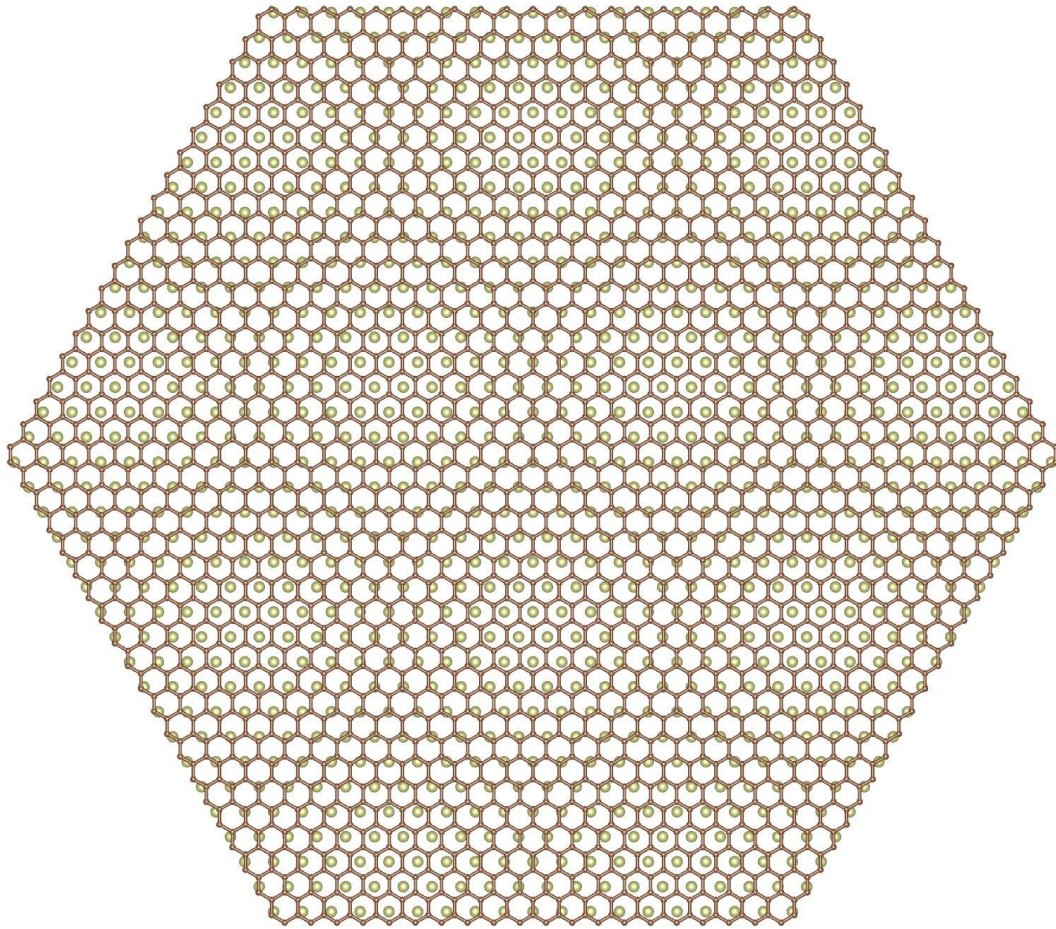


$$I4/mcm \leftarrow P4/mmm \quad P4/mmm \leftarrow Pm3m$$

$$\begin{pmatrix} 1 & 1 & 0 & 1/2 \\ -1 & 1 & 0 & 1/2 \\ 0 & 0 & 2 & 1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

1. Open SrZrO_3 / $\text{SrZrO}_3\text{Perovskite_I4mcm.cif}$
2. Open **Edit Data** dialog, and change to "Keep structure parameters unchanged" mode.
3. Set the above transformation matrix
4. Revert to "Update structure parameters to keep 3D geometry" mode
5. Revert the transformation matrix to identity matrix
6. Set Space group to $Pm3m$, and perform **Remove duplicate atoms**

Practice 5. Align the (111) slice of Ir parallel to graphene

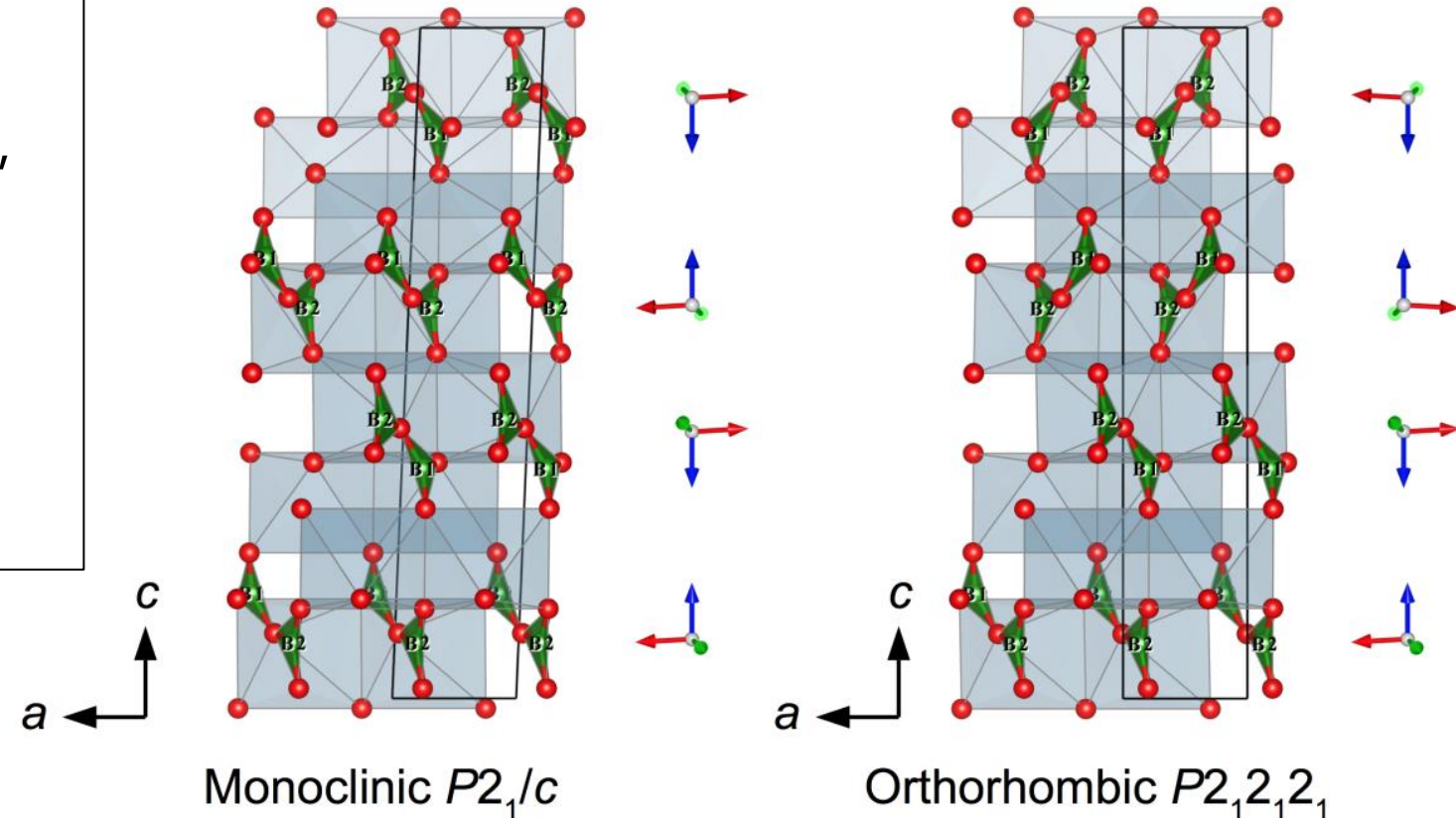


1. Open Ir-graphene/Ir-unitcell.vesta
2. Set **Boundary** as $-9 \leq x, y, z \leq 9$
3. Set Cut off plane and create a slice of (111)
4. Import Ir-graphene/graphite.vesta as 2nd phase
5. Align orientation as
 $[001]_{\text{graphite}} // [111]_{\text{Ir}}, (010)_{\text{graphite}} // (\bar{1}\bar{1}2)_{\text{Ir}}$
6. Set **Boundary** of 2nd phase as
 $-24 \leq x, y \leq 24, 0 \leq z \leq 0.5$

Practice 6. Find possible stacking sequences of polytypes

Background:

- New mineral shimazakiite, (CaB_2O_5), was found.
- Structure of the orthorhombic polytype ($P2_12_12_1$) was first solved.
- Existence of a monoclinic polytype was suggested from TEM observation.

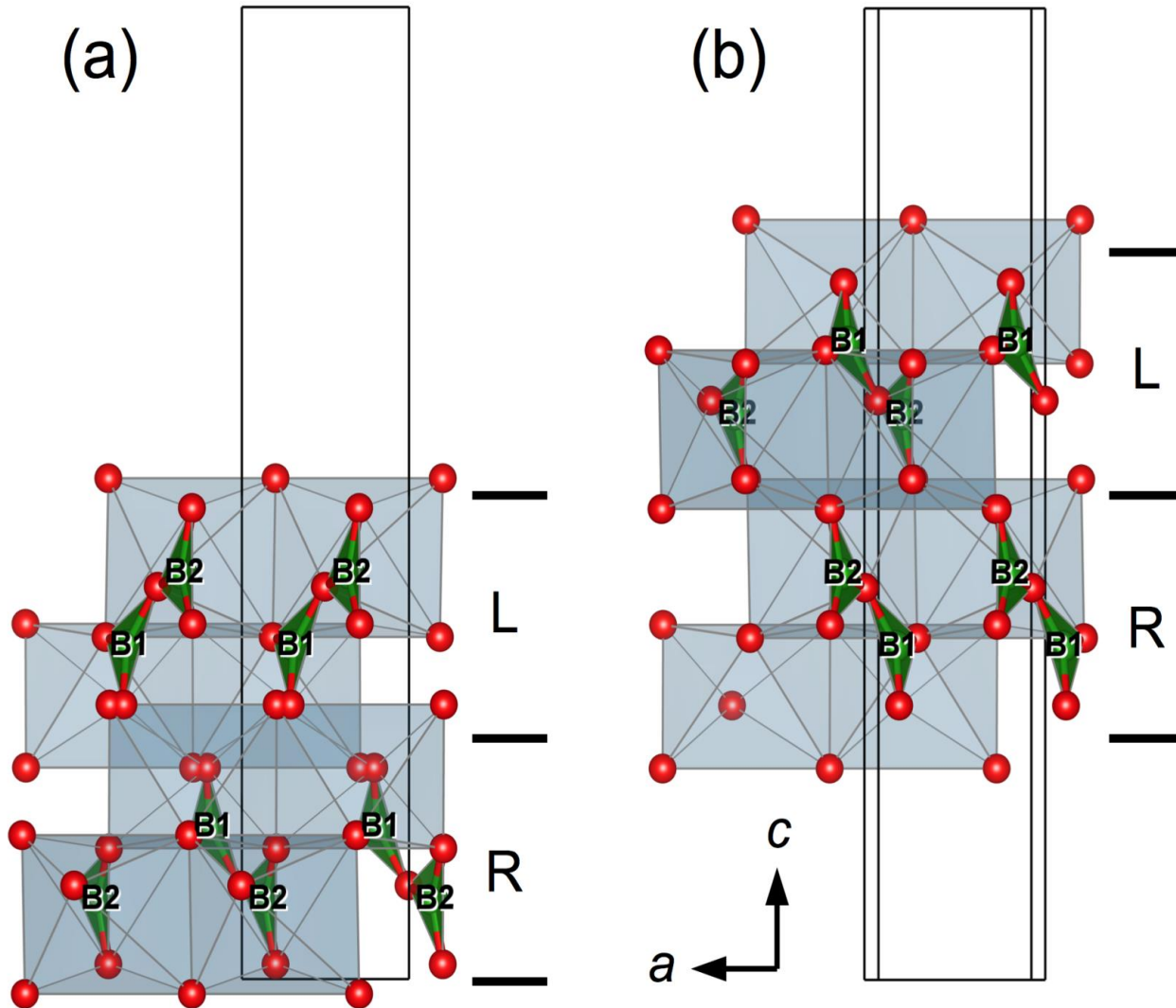


Shimazakiite-4M

Shimazakiite-4O

2 polytypes of shimazakiite (CaB_2O_5)

How layers can be stacked in shimazakiite-4M?

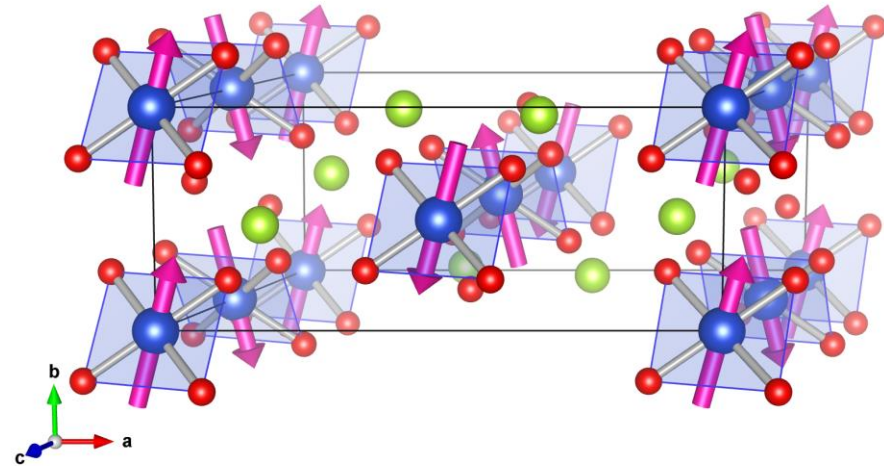
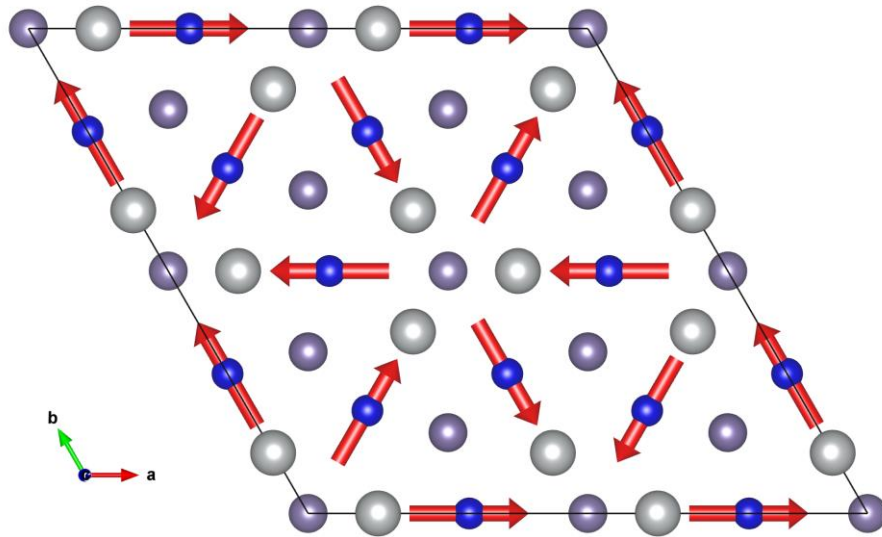


What to do: Starting from 4O structure, create enantiomorphic layer structure, rotate and shift each layer, and find possible stacking positions.

1. Open shimazakiite/shimazakiite-4O.vesta
2. Copy the phase data in **Edit Data** dialog
3. Transform the copied structure to enantiomorphic
4. Set **Boundary** of 1st phase as $\frac{1}{4} \leq z \leq \frac{1}{2}$
5. Set **Boundary** of 2nd phase as $\frac{1}{2} \leq z \leq \frac{3}{4}$
6. Find the best matching position
7. Try other types of staking

Appendix I

Magnetic structures



Magnetic structures

Commensurate structure

1651 magnetic space groups

Incommensurate structure

Magnetic unit cell $\geq$ Crystallographic unit cell

BNS setting

(Belov-Neronova-Smirnova notation)

Based on magnetic unit cell

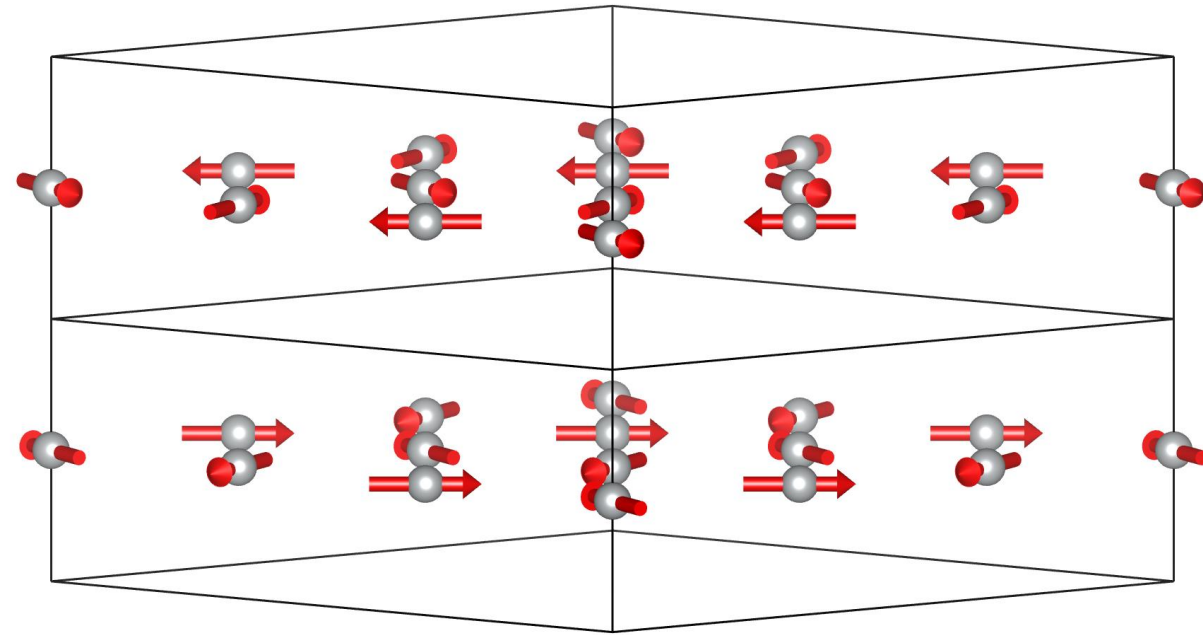
(translation < 1)

OG setting

(Opechowski-Guccione notation)

Based on crystallographic space groups

(translation can be larger than 1)



Magnetic structure of $\text{Ba}_3\text{Nb}_2\text{NiO}_9$

Classification of magnetic space groups

Magnetic space groups derived from $I4_1/amd$

F: Symmetry elements of space group $I4_1/amd$

G: Symmetry elements of magnetic groups

BNS setting		OG setting	
#141.551	$I4_1/amd$	#141.1.1213	$I4_1/amd$
#141.552	$I4_1/amd1'$	#141.2.1214	$I4_1/amd1'$
#141.553	$I4_1/a'md$	#141.3.1215	$I4_1/a'md$
#141.554	$I4_1'/am'd$	#141.4.1216	$I4_1'/am'd$
#141.555	$I4_1'/amd'$	#141.5.1217	$I4_1'/amd'$
#141.556	$I4_1'/a'm'd$	#141.6.1218	$I4_1'/a'm'd$
#141.557	$I4_1/am'd'$	#141.7.1219	$I4_1/am'd'$
#141.558	$I4_1'/a'md'$	#141.8.1220	$I4_1'/a'md'$
#141.559	$I4_1/a'm'd'$	#141.9.1221	$I4_1/a'm'd'$
#141.560	I_c4_1/amd	#134.10.1141	P_14_2/nnm

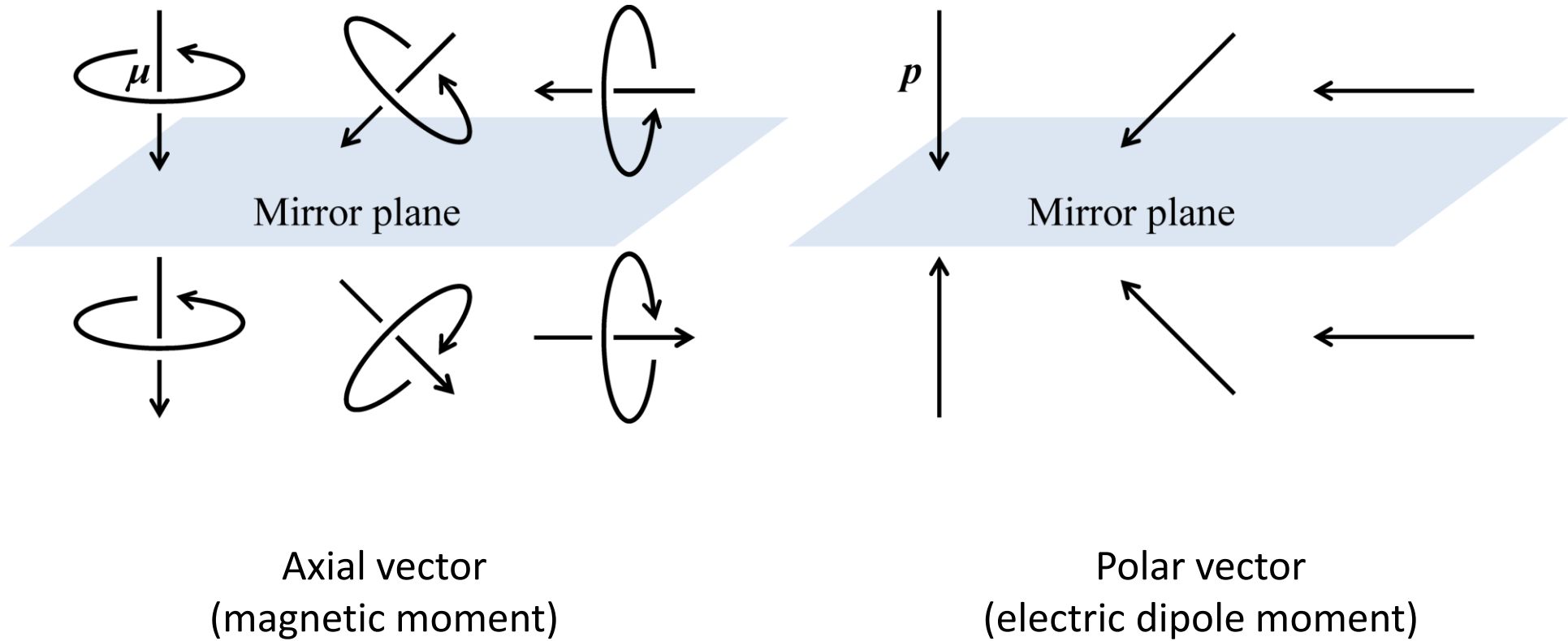
Type 1: $\mathbf{G} = \mathbf{F}$ (Federov group)

Type 2: $\mathbf{G} = \mathbf{F} + \mathbf{F}1'$ (Grey group)

Type 3: $\mathbf{G} = \mathbf{D} + (\mathbf{F} - \mathbf{D})1'$
 (D: Translationgleiche / t-subgroup)
 Translational elements are retained
 but point group is reduced

Type 4: $\mathbf{G} = \mathbf{D} + (\mathbf{F} - \mathbf{D})1'$
 (D: Klassengleiche / k-subgroup)
 Point group is retained but with a
 loss of translations

Axial and polar vectors



Magnetic symmetry operations

$$Q = \begin{pmatrix} Q & q \\ o & 1 \end{pmatrix}$$

$$= \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Diagram labels:

- 3×3 rotation part (points to the Q submatrix)
- 3×1 translation part (points to the q column)
- Time reversal (points to the bottom-right element, 1)

The last row does not contain any information, so we can reuse it to keep time reversal information. When multiplying matrices, however, a special trick is required for not inverting translational component by time reversal operation.

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = Q \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

Atomic coordinates

$$\mu' = |Q| Q \mu$$

Axial vector (μ)
(magnetic moment)

$$p \oplus = Q p$$

Polar vector (p)
(electric dipole moment)

Magnetic space groups

Edit Data - 0.48.mcif

Phase: 1 ▲▼ Tb2 Sn2 O7 ▼

Phase Unit cell Structure parameters Volumetric data Crystal shape

Symmetry

☒ Magnetic structure

System	No.	Space Group	No.	BNS Setting
Molecule	136	P 42/m n m	552	I4_1/amd1 (OG: 141.2.1214 I4_1/amd1)
Custom	137	P 42/n m c	553	I4_1/a'md (OG: 141.3.1215 I4_1/a'md)
Triclinic	138	P 42/n c m	554	I4_1'/am'd (OG: 141.4.1216 I4_1'/am'd)
Monoclinic	139	I 4/m m m	555	I4_1'/amd' (OG: 141.5.1217 I4_1'/amd')
Orthorhombic	140	I 4/m c m	556	I4_1'/a'm'd (OG: 141.6.1218 I4_1'/a'm'd)
Tetragonal	141	I 41/a m d	557	I4_1/am'd' (OG: 141.7.1219 I4_1/am'd')
Trigonal	142	I 41/a c d	558	I4_1'/a'md' (OG: 141.8.1220 I4_1'/a'md')
			559	I4_1/a'm'd' (OG: 141.9.1221 I4_1/a'm'd')

Transform... Customize... Update structure parameters to keep 3D geometry ▲▼

Lattice parameters

	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
	10.42600	10.42600	10.42600	90.0000	90.0000	90.0000
s.u.:	0.00000	0.00000	0.00000	0.0000	0.0000	0.0000

Remove symmetry

Apply Cancel OK

Magnetic symmetry operations

Phase: 1

5yOhtAoR

Rotation matrix (W)

1	0	0
0	1	0
0	0	1

Translation vector (w)

0.000000
0.000000
0.000000

Time reversal (t)

1

General equivalent positions

No.	x'	y'	z'	t	mx'	my'	mz'
1	x	y	z	+1	mx	my	mz
2	-y	x-y+1/2	z	+1	-my	mx-my	mz
3	-x+y+1/2	-x	z	+1	-mx+my	-mx	mz
4	x-y+1/2	-y	-z	+1	mx-my	-my	-mz
5	y	x	-z	+1	my	mx	-mz
6	-x	-x+y+1/2	-z	+1	-mx	-mx+my	-mz
7	-x+y+1/2	-x	-z	-1	-mx+my	-mx	-mz
8	x	y	-z	-1	mx	my	-mz
9	-y	x-y+1/2	-z	-1	-my	mx-my	-mz
10	-x	-x+y+1/2	z	-1	-mx	-mx+my	mz
11	x-y+1/2	-y	z	-1	mx-my	-my	mz
12	y	x	z	-1	my	mx	mz

Close

Symmetry operation $\mathbb{W}$ transforms x, y, z to x', y', z'.

$$\mathbb{W} = \begin{pmatrix} \mathbf{W} & \mathbf{w} \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The (3x3) matrix W is the rotational part.
The (3x1) column matrix w is the translational part.

Transformed coordinates (x', y', z') are related to (x, y, z) by

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

$$= \begin{pmatrix} W_{11}x + W_{12}y + W_{13}z + w_1 \\ W_{21}x + W_{22}y + W_{23}z + w_2 \\ W_{31}x + W_{32}y + W_{33}z + w_3 \\ 1 \end{pmatrix}$$

a **b** **c** **a*** **b*** **c***

 Step (°):
 Step (px):
 Step (%):

Tools Style Objects

V Title

☒ 5yOhtAoR

☒ Atoms

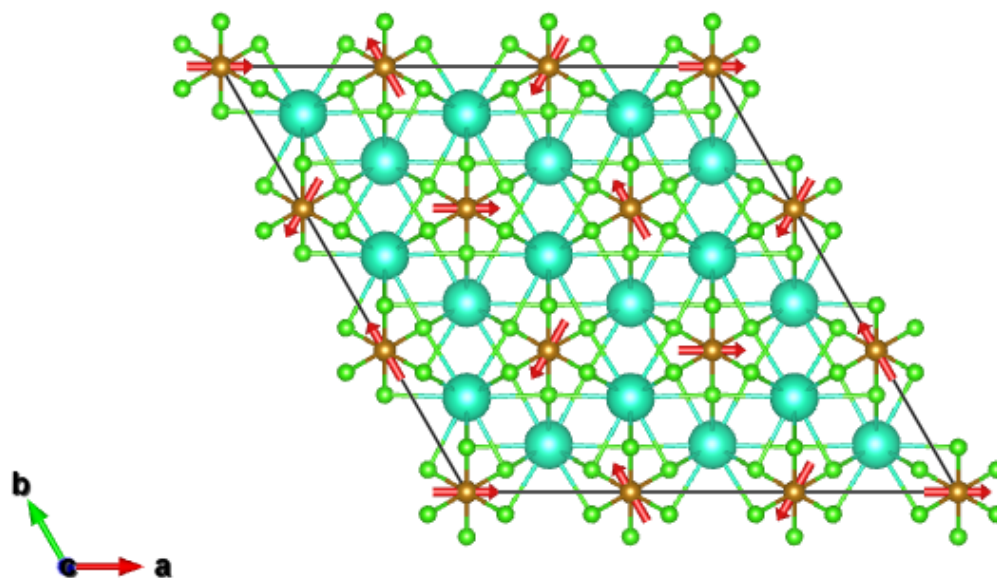
☒ Bonds

☒ Polyhedra

Toggle data: < >

Site	r (Å)	C	L	S	V
☒ Cl	0.99		☐	☐	☒
Cl1	0.99		☐	☐	☒
Cl1_	0.99		☐	☐	☒
Cl1_	0.99		☐	☐	☒
Cl1_	0.99		☐	☐	☒
☒ Fe	1.26		☐	☐	☒
Fe1	1.26		☐	☐	☒
☒ Cs	2.72		☐	☐	☒
Cs1_	2.72		☐	☐	☒
Cs1_	2.72		☐	☐	☒
Cs1_	2.72		☐	☐	☒

Diamond.vesta quartz-kihara.amc xTiO2.vesta 1.0.14_CsFeCl3.mcif



Parent space group name P 6₃/m m c
 Parent space group number 194
 Transformation from parent 3a, 3b, c; 0, 0, 0
 Transformation to parent 1/3a, 1/3b, c; 0, 0, 0
 Magnetic space group name (BNS) P-6'2'm
 Magnetic space group number (BNS) 189.223
 Transformation from standard setting a-b, a+2b, c; 1/3, 1/3, 3/4
 Transformation to standard setting 2/3a+1/3b, -1/3a+1/3b, c; 8/9, 7/9, 1/4

Lattice parameters

Creation of vectors

- Edit → Vectors

Phase: 1 5yOhtAoR

Crystallographic Sites Individual Atom

No.	Label	x	y	z	Vector
1	Tm1_1	0.78800	0.50000	0.50000	
2	Tm1_2	0.28800	0.50000	0.50000	
3	Tm1_3	0.71200	0.50000	0.50000	
4	Ag1_1	0.62500	0.50000	0.50000	
5	Ag1_2	0.12500	0.50000	0.50000	
6	Ag1_3	0.87500	0.50000	0.50000	
7	Ge1_1	0.66667	0.50000	0.50000	
8	Ge1_2	0.83333	0.50000	0.50000	
9	Ge2_1	0.00000	0.50000	0.50000	
10	Ge2_3	0.50000	0.50000	0.50000	

Vectors

No.	[u v w]	Modulus	r (Å)
1	[-0.45830 0.00000 0.00000]	6.44	0.50
4		0.50	
4		0.50	

Edit a Vector

Type: Axial vector Radius: 0.50

Vector components

Lattice vector notation (u, v, w): -0.458298 0 0

Modulus along crystallographic axes: -6.44 0 0

Cartesian vector notation (x, y, z): -6.44 0 0

Modulus: 6.44

☒ Penetrate atoms

☐ Add atom radius to vector modulus

Color: 255 0 0

Length of the vector (automatically calculated)

Scale factor for modulus: 0.232919

Scale factor

3 types of representations
(u, v, w)
(ma, mb, mc)
(x, y, z)

Cancel OK