Crystallographic Symmetry Computations

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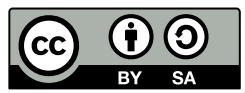


Contents of this talk

1. Introduce some notation;
2. Introduce definition of a crystal and crystal lattice;
3. Show how symmetry operations are described;
4. Describe crystallographic coordinate transformations;
5. Show some computer code dealing with crystal symmetry;

With this talk I intend to help the participants:

- to become more familiar with crystallographic coordinate transformations,
- to be able to apply crystal symmetry operations;
- to be able to write simple computer code that handles crystallographic symmetry and atomic coordinates.

Notation

x, y, z	scalars, vector components, integers, reals, ...
$\mathbf{v}, \vec{v}$	vectors
$(\mathbf{a} \cdot \mathbf{b})$	scalar product of **a** and **b**
$(\mathbf{a} \times \mathbf{b})$	cross-product product of **a** and **b**
$\mathrm{A}, \mathrm{B}, \mathrm{C}$	linear operators A, B and C
$\mathrm{A}\mathbf{v}$	application of a linear operator to a vector
$\mathrm{AB};\ \ (\mathrm{AB})\mathbf{v} \stackrel{def}{=} \mathrm{A}(\mathrm{B}\mathbf{v})$	product of two linear operators
$B = [\mathbf{a}, \mathbf{b}, \mathbf{c}]$	basis B consisting of vectors **a**, **b** and **c**
$[\mathbf{a}]_B = [a_i]_B = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}_B$	a column vector in basis B with components a_1, a_2, a_3
$\mathrm{A} = [a_{ij}]_B = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix}_B$	linear operator represented as matrix in basis B
$[\mathbf{a}]_O = [a_i]_O$	vector **a** in an orthonormal (Cartesian) frame O
$\mathrm{A}^T, [a_{ij}]^T, [v_i]^T = [v_1, \dots, v_N]$	transpose matrices and vectors

Notation examples

- vector $\mathbf{x}$ can be expressed using components in the basis $B = [\mathbf{e}_i]$:
  $\mathbf{x} = [\mathbf{e}_i]^T [x_i]_B = \sum_{i=1}^{N} x_i \mathbf{e}_i = [\mathbf{a}, \mathbf{b}, \mathbf{c}] [x_i]_B = x_1 \mathbf{a} + x_2 \mathbf{b} + x_3 \mathbf{c}$
  (last 2 eqns. — in case of 3D space ($N = 3$))

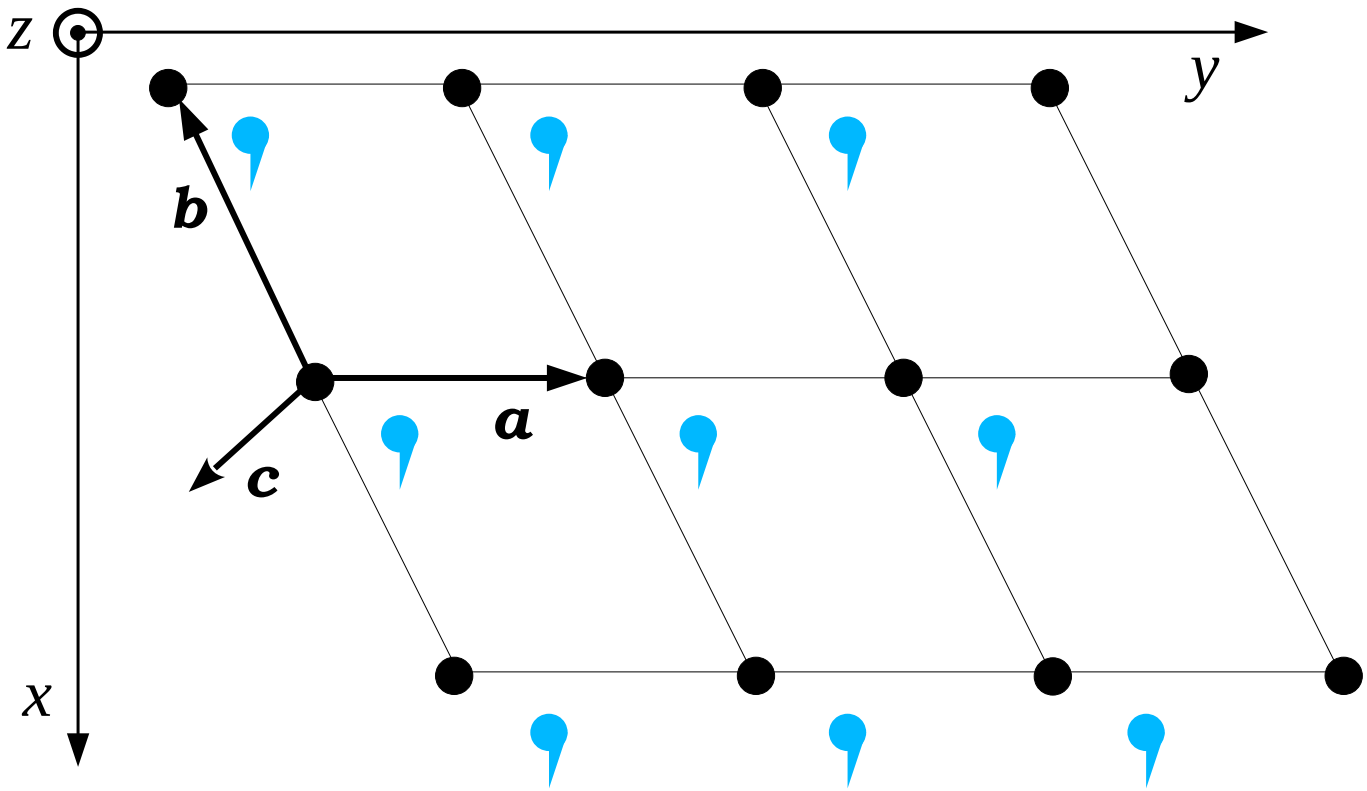
- Scalar product is especially simple in Cartesian frame:

$$(\mathbf{x} \cdot \mathbf{y}) = [x_i]_O^T [y_i]_O = [x_1, x_2, \ldots, x_N]_O \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}_O = \sum_{i=1}^{N} x_i y_i$$

- need more work in a non-orthogonal frame $B = [\mathbf{a}, \mathbf{b}, \mathbf{c}]$:

$$\begin{aligned} (\mathbf{x} \cdot \mathbf{y}) &= ([\mathbf{a}, \mathbf{b}, \mathbf{c}] [x_i]_B \cdot [\mathbf{a}, \mathbf{b}, \mathbf{c}] [y_i]_B) \\ &= ([\mathbf{a}, \mathbf{b}, \mathbf{c}]_O [x_i]_B)^T [\mathbf{a}, \mathbf{b}, \mathbf{c}]_O [y_i]_B \\ &= [x_i]_B^T ([\mathbf{a}, \mathbf{b}, \mathbf{c}]_O^T [\mathbf{a}, \mathbf{b}, \mathbf{c}]_O) [y_i]_B \end{aligned}$$

Definition of a crystal

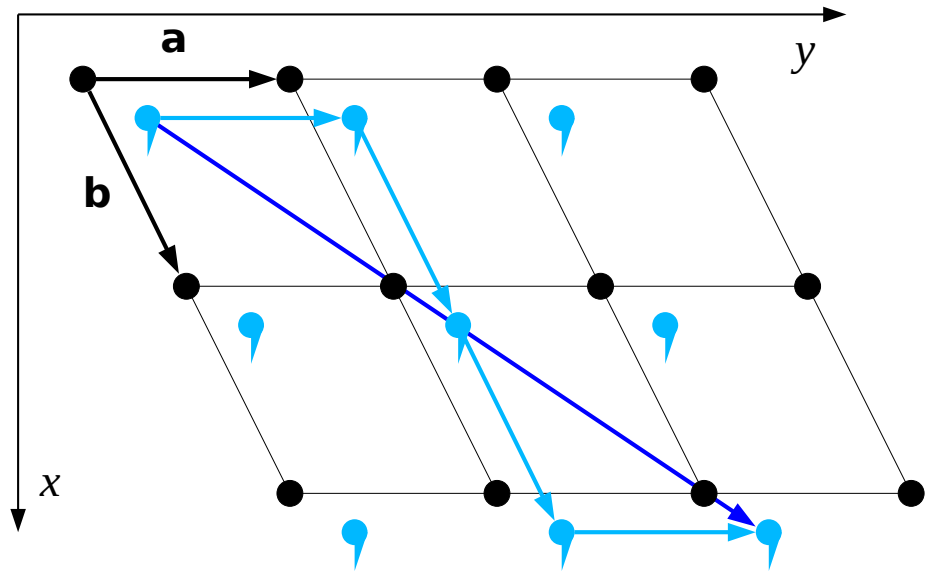


Any translation expressed by:

$$\mathbf{T}_{p,q,r} = p\,\mathbf{a} + q\,\mathbf{b} + r\,\mathbf{c},\ p, q, r \in \mathbb{Z}$$

maps the crystal to itself.

The crystal translation group

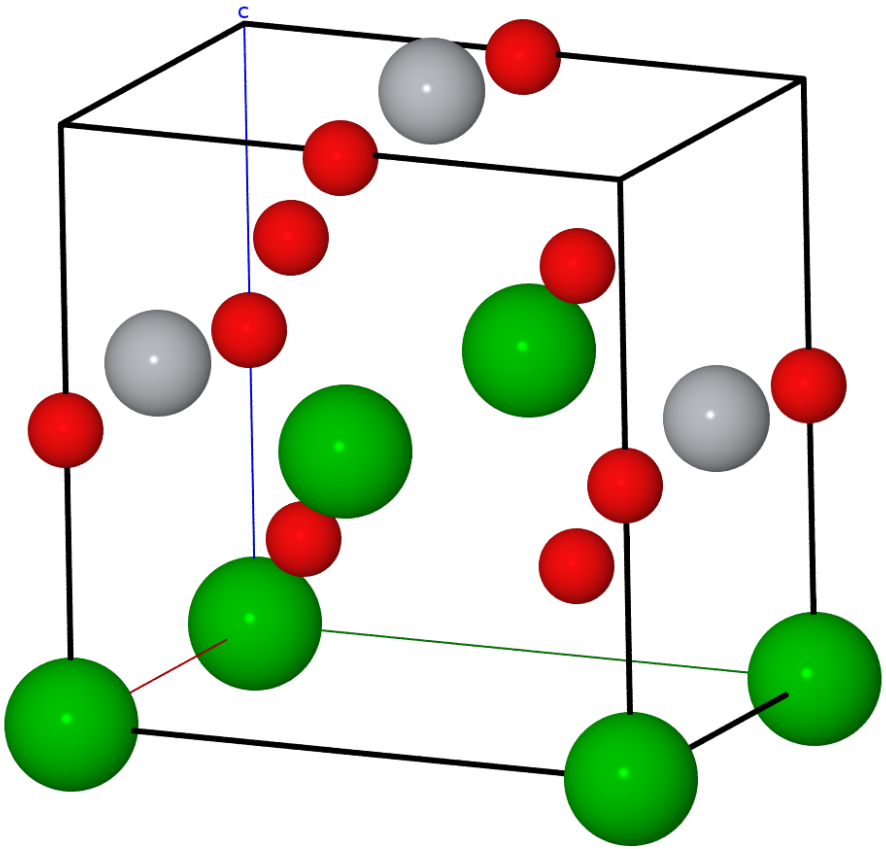


All translations $\mathbf{T}_{p,q,r}$ form a commutative group $\mathbb{T}$:

- $\forall\, p, q, r,\ k, l, m \in \mathbb{Z}$: $\quad \mathbf{T}_{p,q,r} + \mathbf{T}_{k,l,m} = \mathbf{T}_{p+k,q+l,r+m} \in \mathbb{T}$;
- $\exists\, \mathbf{0} = \mathbf{T}_{0,0,0} \in \mathbb{T}$: $\ \forall\, \mathbf{T}_{p,q,r} \in \mathbb{T}$: $\quad \mathbf{T}_{p,q,r} + \mathbf{0} = \mathbf{T}_{p,q,r}$;
- $\exists\, -\mathbf{T}_{p,q,r} = \mathbf{T}_{-p,-q,-r}$: $\quad \mathbf{T}_{p,q,r} + (-\mathbf{T}_{p,q,r}) = \mathbf{0}$;

The lattice and the unit cell

COD entry 9014492:



(Kwei et al. 1993)

The lattice and the unit cell

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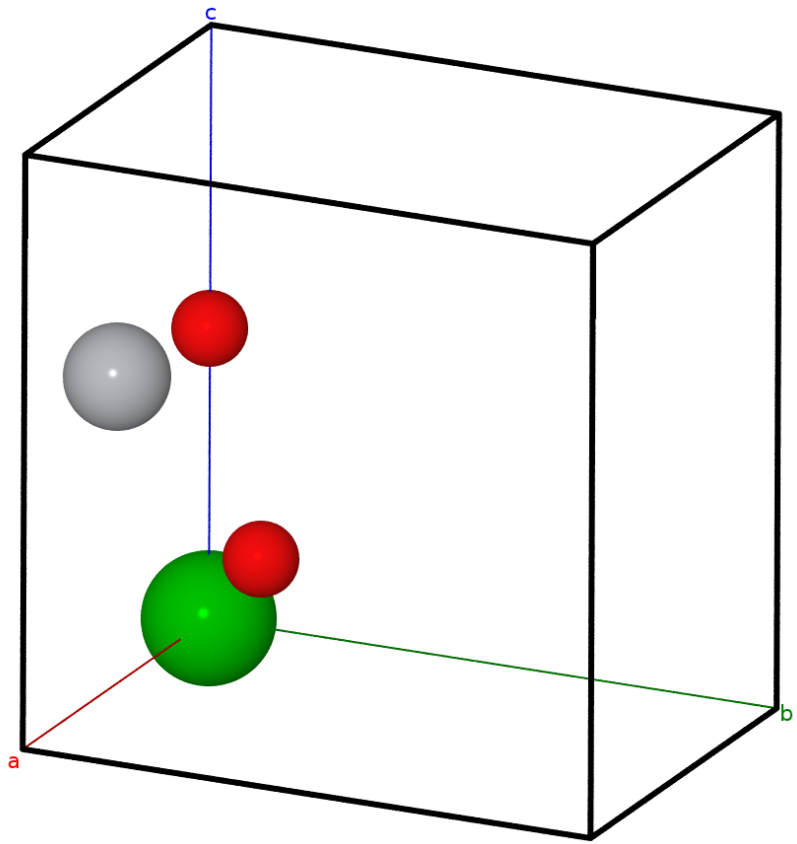
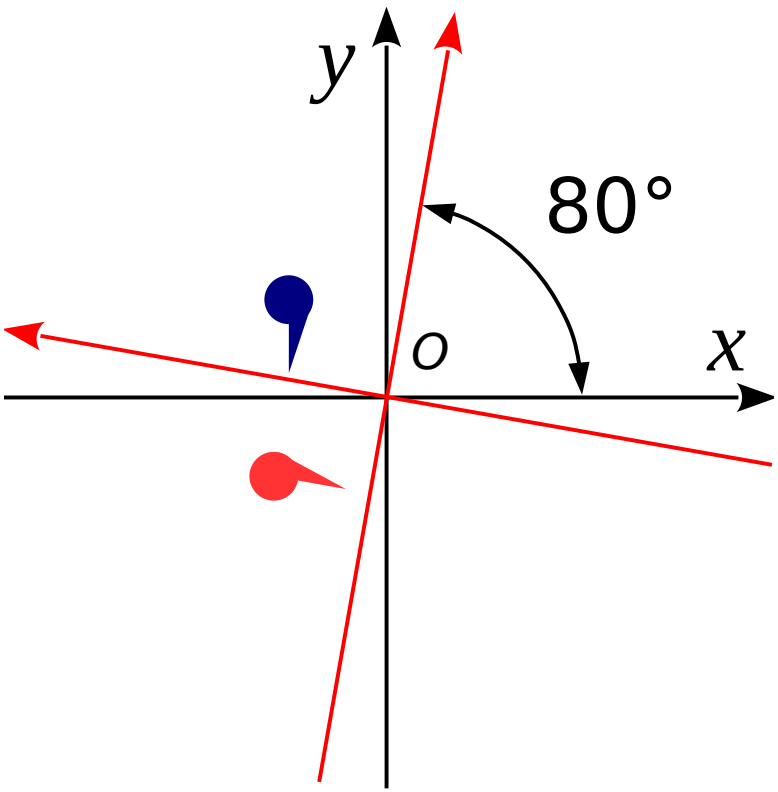


(Kwei et al. 1993)

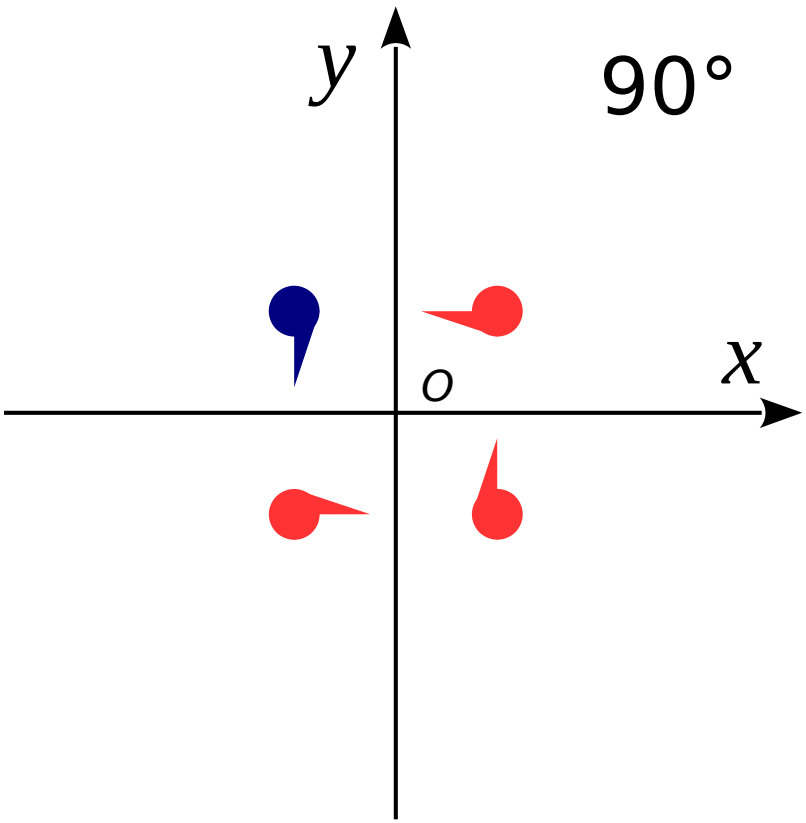
Point symmetry

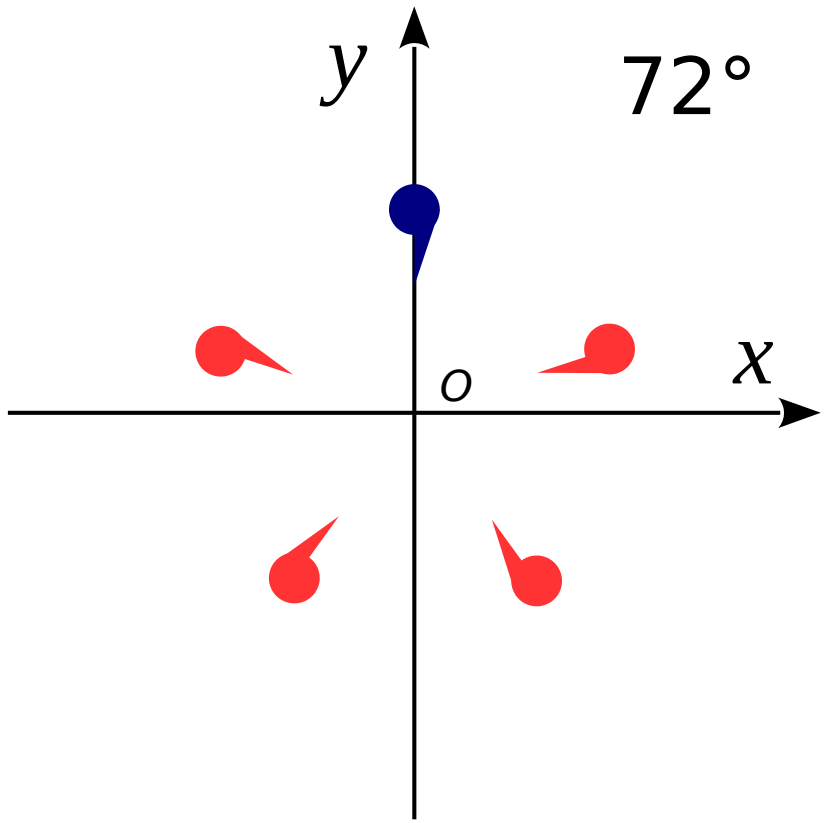


$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}_O = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}_O$$

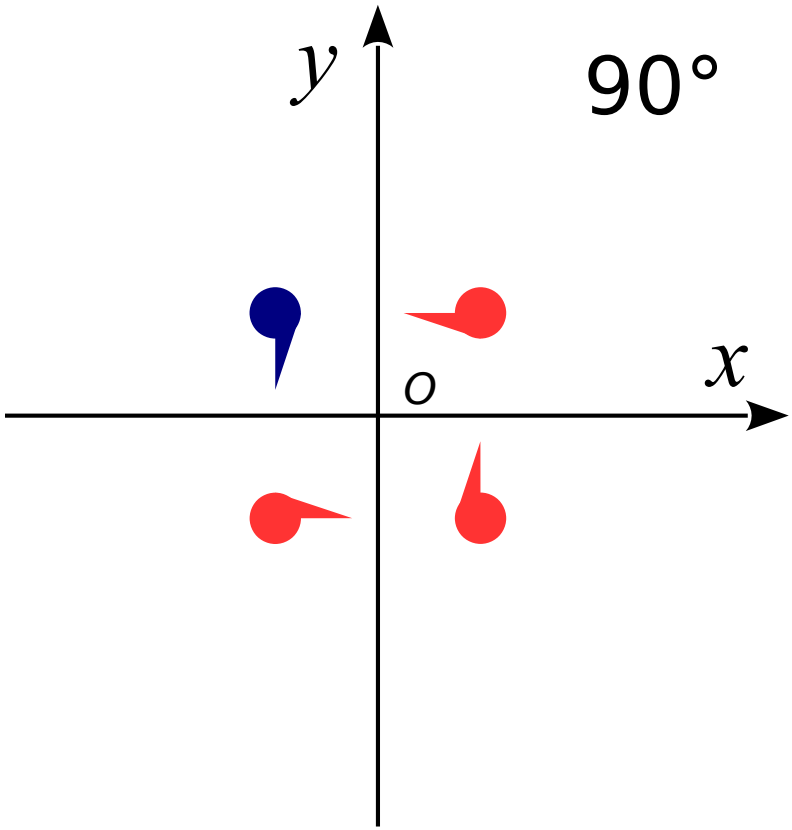
$$[x_i'] = \mathrm{R}_\phi [x_i]$$

Point group





Point group



$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$\begin{bmatrix} x'' \\ y'' \\ z'' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$\begin{bmatrix} x''' \\ y''' \\ z''' \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

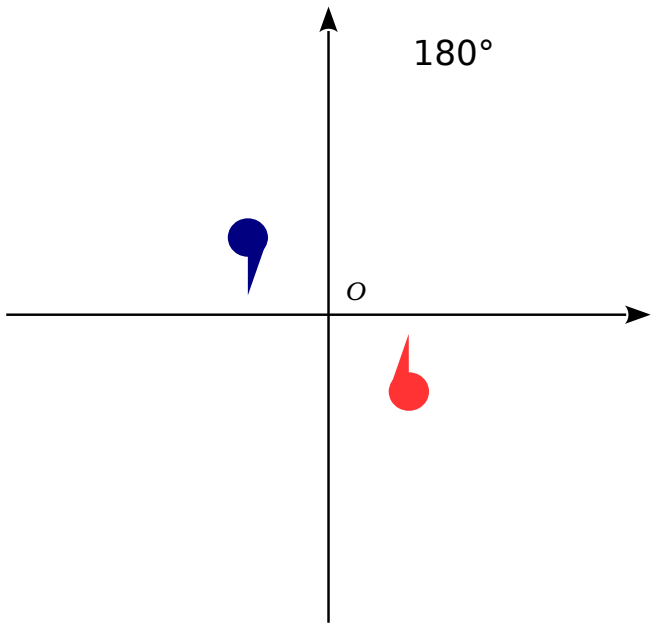
$$\begin{bmatrix} x^{(4)} \\ y^{(4)} \\ z^{(4)} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Description of symmetry operations

Coordinates of a general position:

$$-x, -y, z + \frac{1}{2}$$

("Jones's faithful notation")



Rotation matrix + translation:

$$\mathbf{x}' = \mathrm{R}\mathbf{x} + \mathbf{T}$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} t_x \\ t_y \\ t_z \end{bmatrix}$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0.5 \end{bmatrix}$$

Isometries

Definition

Isometry is a mapping of Euclidean space to itself that does not change distance between mapped ponts.

Theorem

An isometry is a linear mapping (operator). Its matrix prepresentation in a Cartesian frame of reference is an orthogonal matrix.

Isometries

Theorem

An isometry is a linear mapping (operator). Its matrix prepresentation in a Cartesian frame of reference is an orthogonal matrix.

Proof.

"Does not change distance" $\equiv$ "Preserves scalar product"; i.e.:

$$(\mathbf{x} \cdot \mathbf{y}) = (\mathrm{R}\mathbf{x} \cdot \mathrm{R}\mathbf{y}) = (\mathrm{R}_O [\mathbf{x}]_O)^T \cdot \mathrm{R}_O [\mathbf{y}]_O = [\mathbf{x}]_O \mathrm{R}_O^T \mathrm{R}_O [\mathbf{y}]_O$$

since the equality must hold for *any* $\mathbf{x}$ and $\mathbf{y}$,

$$\Rightarrow \mathrm{R}_O^T \mathrm{R}_O = \mathrm{I}$$

Orthogonal matrices

Properties of orthogonal matrices

Orthogonal matrices have columns (and rows) orhonormal:

$$[r_{ij}]_O = [\mathbf{r}_1, \ldots, \mathbf{r}_N]_O = \begin{bmatrix} r_{11} & \ldots & r_{1N} \\ \vdots & \ddots & \vdots \\ r_{N1} & \ldots & r_{NN} \end{bmatrix}_O$$

such that

$$(\mathbf{r}_i \cdot \mathbf{r}_j) = \delta_{ij} \; \forall \, i,j = 1 \ldots N$$

Proper and improper rotations

Determinant of an orthogonal matrix

$$\mathrm{R}^T\mathrm{R} = \mathrm{I} \Rightarrow$$
$$\det(\mathrm{R}^T\mathrm{R}) = \det \mathrm{I}$$

at the same time,

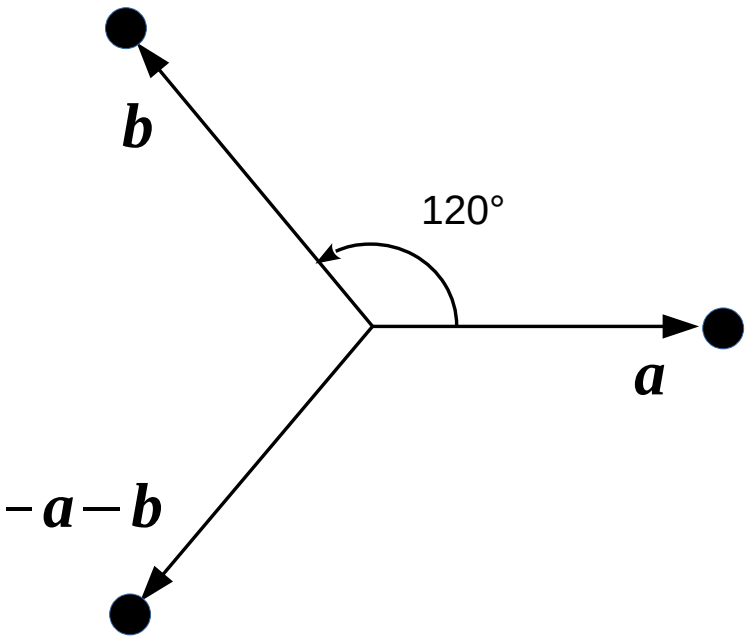
$$\det(\mathrm{R}^T\mathrm{R}) = \det \mathrm{R}^T \cdot \det \mathrm{R} =$$
$$\det \mathrm{R} \cdot \det \mathrm{R} = (\det R)^2 = 1$$

therefore,

$$\det R = 1 \vee \det R = -1$$

1. $\det R = 1$ – (proper) rotations;
2. $\det R = -1$ – improper rotations (reflections);

Rotation matrices in different frames



Orthogonal basis:

$$\mathrm{R}_{120^\circ} = \begin{bmatrix} \cos 120^\circ & -\sin 120^\circ & 0 \\ \sin 120^\circ & \cos 120^\circ & 0 \\ 0 & 0 & 1 \end{bmatrix}_O$$

"Natural" basis
(fractional coords):

$$\mathrm{R}_{120^\circ} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}_B$$

$$[\mathrm{R}_\phi]_B = \mathrm{S}\,[\mathrm{R}_\phi]_O\,\mathrm{S}^{-1}$$

Trace of a matrix

$$R = \begin{bmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\Rightarrow$$

$$\mathrm{Tr}\ \mathrm{R} \in \mathbb{Z}$$

$$R = \begin{bmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\Rightarrow$$

$$\mathrm{Tr}\ \mathrm{R} = 2\cos\phi + 1 \in \mathbb{Z}$$
$$\phi \in \{60°, 90°, 120°, 180°\}$$

Combinations of symmetry elements

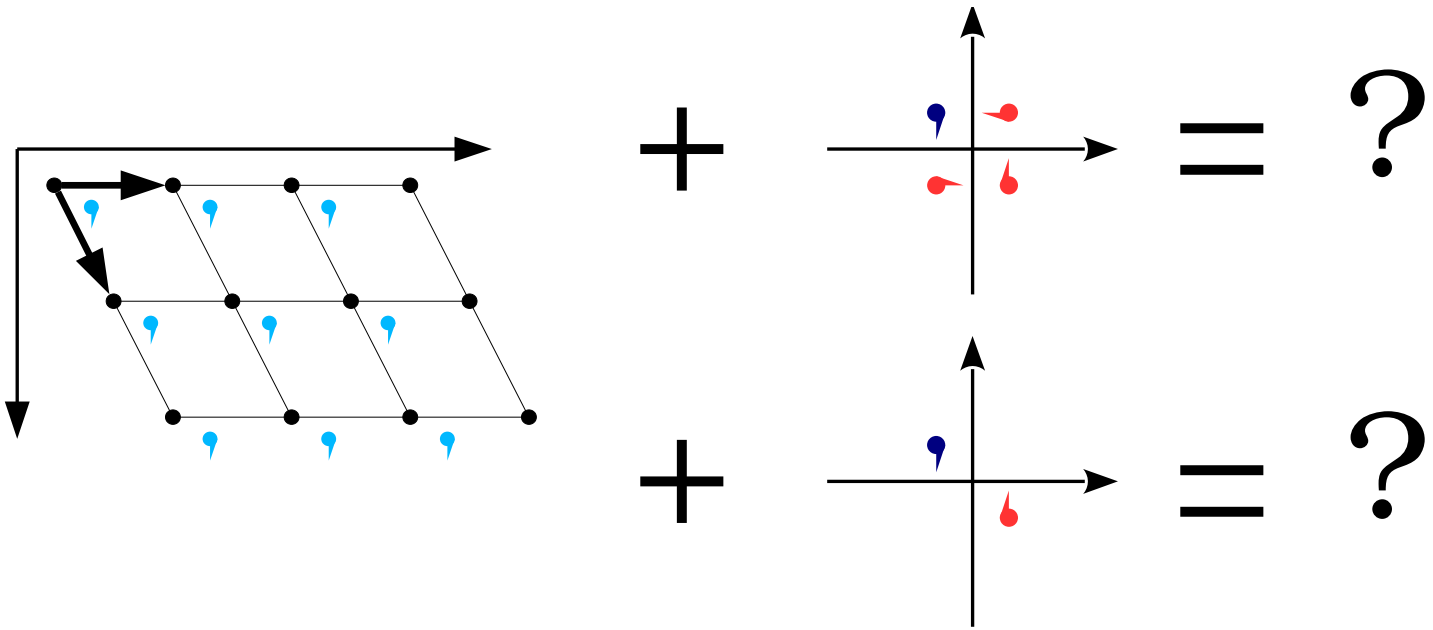
$$\vec{x}' = R\vec{x} + \vec{T}$$
$$\vec{x}'' = R'(R\vec{x} + \vec{T}) + \vec{T}' =$$
$$= R'R\vec{x} + R'\vec{T} + \vec{T}'$$

$$S = R + \vec{T}\,; S' = R' + \vec{T}'$$
$$S'S = R'R + (R'\vec{T} + \vec{T}')$$

$$R'R = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$-x, -y, z$ $\quad$ $-x, y, -z$ $\quad$ $x, -y, -z$

Symmetry elements compatible with the lattice



230 space groups

The number of space groups is *finite* in any dimensions (17 in 2D, 230 in 3D)

Nomenclature:

- Schönflies symbols: C_{5h}, D_6, ...
- ITC numbers: $1, 2, \ldots, 230$:)
- Hermann-Mauguin symbols: $C\,2$, $P\,2_1\,2_1\,2_1$, ...
- Hall symbols: `P 2xa`, `I -2c -2c`, ...

Factorising a space group

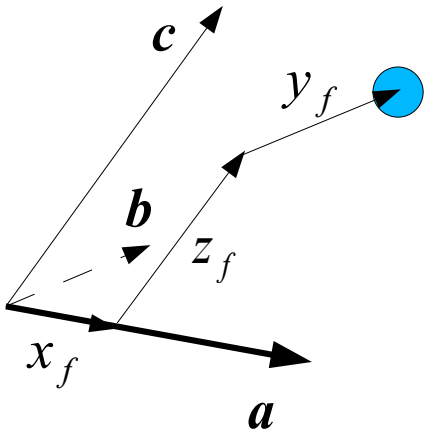
- The crystal translation group is a *normal* subgroup of a space group;
- we can factorise the space group with respect to this normal subgrup (i.e. declare al translated symmetry operations to be equivalent);
- the factorgroup is finite;

Crystallographic coordinate frames

Fractional and Cartesian coordinates

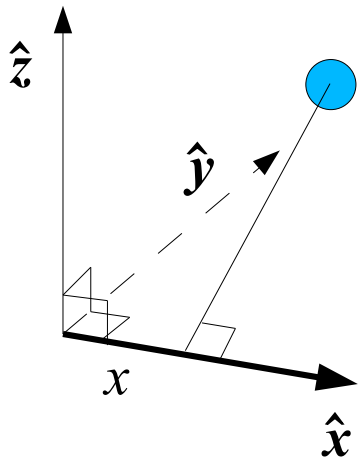
Fractional

(as fractions of unit cell vectors)

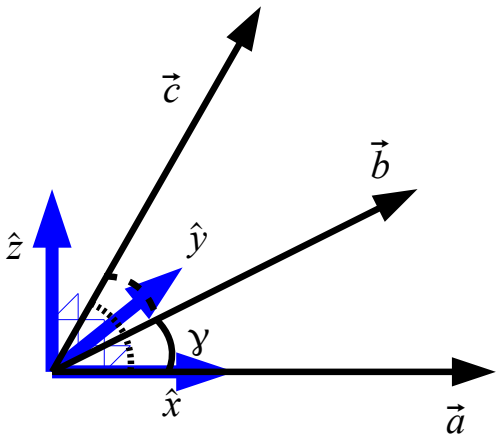


Cartesian (orthonormal)

In an orthonormal basis (coordinate system)



Coordinate transformations



$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \qquad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} a_x & b_x & c_x \\ 0 & b_y & c_y \\ 0 & 0 & c_z \end{bmatrix} \begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix}$$

Senosios bazės komponentės naujoje bazėje

$$\vec{\boldsymbol{x}} = \boldsymbol{E}' \vec{\boldsymbol{x}}' \qquad \boldsymbol{E}' = \begin{bmatrix} e_{1x} & e_{2x} & e_{3x} \\ e_{1y} & e_{2y} & e_{3y} \\ e_{1z} & e_{2z} & e_{3z} \end{bmatrix}$$

$$\vec{\boldsymbol{x}}' = \boldsymbol{E} \vec{\boldsymbol{x}}$$

$$\boldsymbol{E}' = \boldsymbol{E}^{-1};\ \boldsymbol{E} \cdot \boldsymbol{E}' = \boldsymbol{I}$$

$$(\vec{\boldsymbol{x}}_1 \cdot \vec{\boldsymbol{x}}_2) = \vec{x}_1^{\,T} \vec{x}_2 = x_1 x_2 + y_1 y_2 + z_1 z_2 =$$
$$= (\vec{\boldsymbol{x}}_1' \cdot \vec{\boldsymbol{x}}_2') =$$
$$= \vec{x}_1'^{\,T} E'^{T} E' \vec{x}_2'$$

Orthogonalisation convention

The SCALEn (n = 1, 2, or 3) records present the transformation from the orthogonal coordinates as contained in the entry to fractional crystallographic coordinates.

If the orthogonal Angstroms coordinates are X, Y, Z, and the fractional cell coordinates are xfrac, yfrac, zfrac, then:

xfrac = S11X + S12Y + S13Z + U1
yfrac = S21X + S22Y + S23Z + U2
zfrac = S31X + S32Y + S33Z + U3

$$\begin{bmatrix} x_f \\ y_f \\ z_f \end{bmatrix} = \begin{bmatrix} x_a & y_a & z_a \\ 0 & y_b & z_b \\ 0 & 0 & z_c \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

Conversion between frames

Perl

$$\mathbf{x}' = \mathrm{R}\mathbf{x} + \mathbf{T}_0$$

```
sub symop_ortho_from_fract
{
    my @cell = @_;
    my ($a, $b, $c) = @cell[0..2];
    my ($alpha, $beta, $gamma) = map {$Pi * $_ / 180} @cell[3..5];
    my ($ca, $cb, $cg) = map {cos} ($alpha, $beta, $gamma);
    my $sg = sin($gamma);

    return [
        [ $a, $b*$cg, $c*$cb                    ],
        [  0, $b*$sg, $c*($ca-$cb*$cg)/$sg ],
        [  0,      0,
              $c*sqrt($sg*$sg-$ca*$ca-$cb*$cb+2*$ca*$cb*$cg)/$sg ]
    ];
}
```

Conversion between frames

Ada

$$\mathbf{x}' = \mathrm{R}\mathbf{x} + \mathbf{T}_0$$

```
function Matrix_Ortho_From_Fract ( Cell : Unit_Cell_Type ) return Matrix3x3
   is
      A : Long_Float := Cell(1);
      B : Long_Float := Cell(2);
      C : Long_Float := Cell(3);
      Alpha : Long_Float := Cell(4) * Ada.Numerics.Pi / 180.0; -- in radians;
      Beta  : Long_Float := Cell(5) * Ada.Numerics.Pi / 180.0;
      Gamma : Long_Float := Cell(6) * Ada.Numerics.Pi / 180.0;
      CA : Long_Float := Cos(Alpha);
      CB : Long_Float := Cos(Beta);
      CG : Long_Float := Cos(Gamma);
      SG : Long_Float := Sin(Gamma);
   begin
      return (
                (   A, B * CG, C * CB                    ),
                ( 0.0, B * SG, C * (CA - CB*CG) / SG ),
                ( 0.0,    0.0, C * Sqrt (SG*SG - CA*CA - CB*CB + 2.0*CA*CB*CG)/SG)
              );
   end;
```

Distances & Metric tensor

$$G = E'^{T} E'$$

$$G = E'^{T} E' = \begin{bmatrix} e_{1x} & e_{1y} & e_{1z} \\ e_{2x} & e_{2y} & e_{2z} \\ e_{3x} & e_{3y} & e_{3z} \end{bmatrix} \begin{bmatrix} e_{1x} & e_{2x} & e_{3x} \\ e_{1y} & e_{2y} & e_{3y} \\ e_{1z} & e_{2z} & e_{3z} \end{bmatrix} = \begin{bmatrix} (\vec{e}_1 \cdot \vec{e}_1) & (\vec{e}_1 \cdot \vec{e}_2) & (\vec{e}_1 \cdot \vec{e}_3) \\ (\vec{e}_2 \cdot \vec{e}_1) & (\vec{e}_2 \cdot \vec{e}_2) & (\vec{e}_2 \cdot \vec{e}_3) \\ (\vec{e}_3 \cdot \vec{e}_1) & (\vec{e}_3 \cdot \vec{e}_2) & (\vec{e}_3 \cdot \vec{e}_3) \end{bmatrix}$$

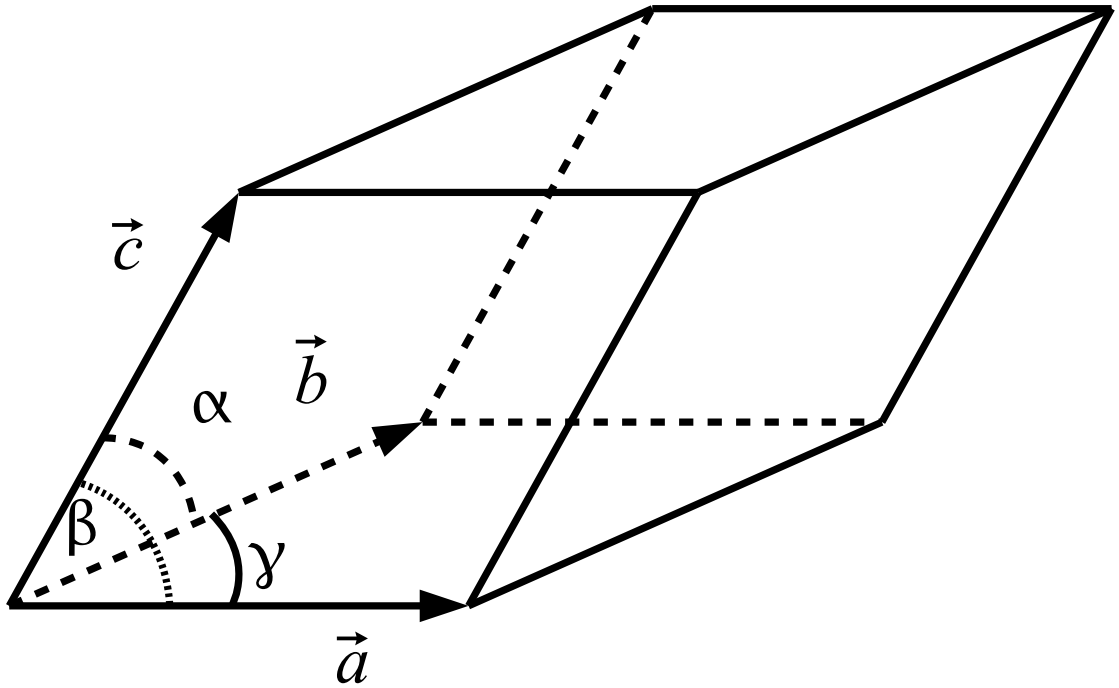
$$G = G^{T}$$

$$G = \begin{bmatrix} (\vec{a} \cdot \vec{a}) & (\vec{a} \cdot \vec{b}) & (\vec{a} \cdot \vec{c}) \\ (\vec{b} \cdot \vec{a}) & (\vec{b} \cdot \vec{b}) & (\vec{b} \cdot \vec{c}) \\ (\vec{c} \cdot \vec{a}) & (\vec{c} \cdot \vec{b}) & (\vec{c} \cdot \vec{c}) \end{bmatrix}$$

$$(\vec{x}_1 \cdot \vec{x}_2) = \vec{x}_1^{\,T} G \, \vec{x}_2$$

Volume of a unit cell

$$V = (\vec{a} \cdot [\vec{b} \times \vec{c}]) = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} = \sqrt{|det\, G|}$$



Determinant of a metric tensor

$$[\vec{b}\times\vec{c}]=\begin{vmatrix}\hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}}\\ b_x & b_y & b_z\\ c_x & c_y & c_z\end{vmatrix}=\hat{\mathbf{x}}(b_y c_z-b_z c_y)+\hat{\mathbf{y}}\ldots$$

$$V=(\vec{a}\cdot[\vec{b}\times\vec{c}])=a_x(b_y c_z-b_z c_y)+a_y\ldots=\begin{vmatrix}a_x & a_y & a_z\\ b_x & b_y & b_z\\ c_x & c_y & c_z\end{vmatrix}=$$

$$=det\,E'^{T}=det\,E'$$

$$det\,G=det\,(E'^{T}E)=det\,(E'^{T})\,det\,(E')=(det\,E')^2$$

$$V=(\vec{a}\cdot[\vec{b}\times\vec{c}])=det\,(E')=\sqrt{|det\,G|}$$

New cell invariant (V. Kurlin's group)

Point-wise Distance Distributions

- Since a PDD is just a particular arrangement of inter-point distances, it's an *invariant* (1) independent of any choice of cell and motif.
- Given a proper *metric* (4) between PDDs (*Earth mover's distance*), it's *continuous* (3) even if symmetries break under perturbation.
- PDDs are *computable* (5) in near-linear time in the motif size and k, and performs well practically ($\sim$1ms/structure for $k = 100$).
- PDDs are *almost complete* (2). Our group have worked on complete invariants; the PDD sacrifices *some* completeness in exchange for simplicity and speed. Incompleteness is proven to occur only on a 'small' (measure zero) part of crystal space. Where it is complete, crystals can even be *reconstructed* from their PDD.

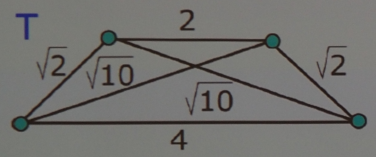
13/28

(Widdowson and Kurlin 2023), IUCr26

Continuous crystal similarity measure

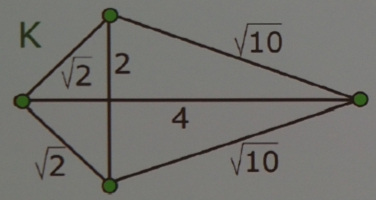
Simple example of PDD strength

Minimal example of how the PDD contains more information than a simple list of inter-point distances:



$$\longrightarrow \quad \mathrm{PDD}(T;3) = \left(\begin{array}{c|ccc} 1/2 & \sqrt{2} & 2 & \sqrt{10} \\ 1/2 & \sqrt{2} & \sqrt{10} & 4 \end{array}\right)$$

$$\neq$$



$$\longrightarrow \quad \mathrm{PDD}(K;3) = \left(\begin{array}{c|ccc} 1/4 & \sqrt{2} & \sqrt{2} & 4 \\ 1/2 & \sqrt{2} & 2 & \sqrt{10} \\ 1/4 & \sqrt{10} & \sqrt{10} & 4 \end{array}\right)$$

14/28

(Widdowson and Kurlin 2023), IUCr26

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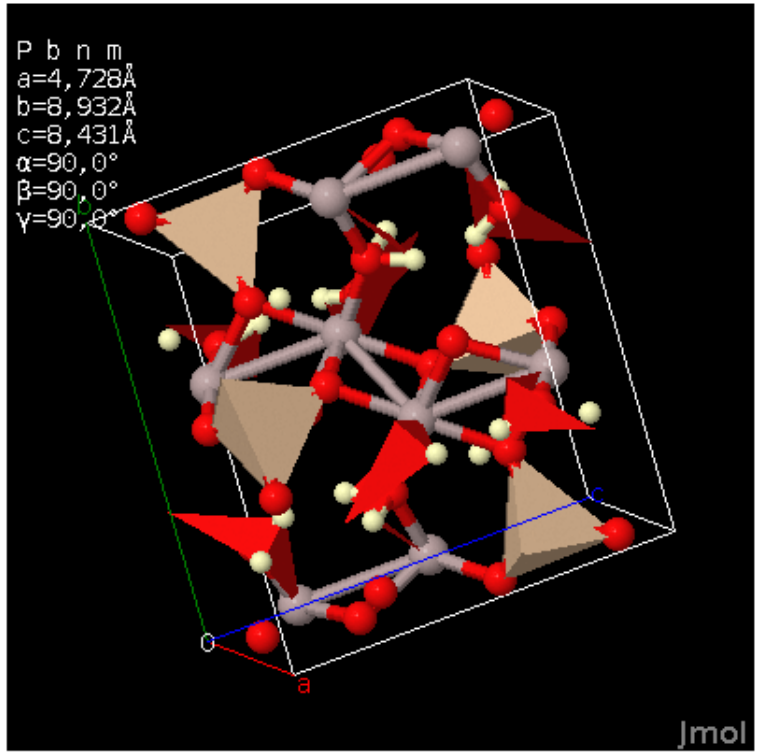
Thank you!



Coordinates	2207377.cif
Original IUCr paper	HTML

http://en.wikipedia.org/wiki/Topaz

http://www.crystallography.net/2207377.html

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Glazer, A. Michael et al. (Mar. 2014). "Seitz symbols for crystallographic symmetry operations". In: *Acta Crystallographica Section A Foundations and Advances* 70.3, pp. 300–302. DOI: 10.1107/s2053273314004495.

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