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CRYSTALLOGRAPHIC SYMMETRY OPERATIONS

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SYMMETRY OPERATIONS
AND
THEIR MATRIX-COLUMN
PRESENTATION
**Mappings and symmetry operations**

**Definition:** A mapping of a set $A$ into a set $B$ is a relation such that for each element $a \in A$ there is a unique element $b \in B$ which is assigned to $a$. The element $b$ is called the *image* of $a$.

The relation of the point $X$ to the points $\tilde{X}_1$ and $\tilde{X}_2$ is not a mapping because the image point is not uniquely defined (there are two image points).

The five regions of the set $A$ (the triangle) are mapped onto the five separated regions of the set $B$. No point of $A$ is mapped onto more than one image point. Region 2 is mapped on a line, the points of the line are the images of more than one point of $A$. Such a mapping is called a projection.
Definition: A **mapping** of a set $A$ into a set $B$ is a relation such that for each element $a \in A$ there is a unique element $b \in B$ which is assigned to $a$. The element $b$ is called the **image** of $a$.

An **isometry** leaves all distances and angles invariant. An ‘isometry of the first kind’, preserving the counter–clockwise sequence of the edges ‘short–middle–long’ of the triangle is displayed in the upper mapping. An ‘isometry of the second kind’, changing the counter–clockwise sequence of the edges of the triangle to a clockwise one is seen in the lower mapping.

A parallel shift of the triangle is called a **translation**.Translations are special isometries. They play a distinguished role in crystallography.
Example: Matrix presentation of symmetry operation

Mirror symmetry operation

Mirror line $m_y$ at 0,y

Matrix representation

Fixed points

$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x \\ y \end{bmatrix}$

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

$\det \begin{bmatrix} -1 & \phantom{1} \\ 1 & \phantom{1} \end{bmatrix} = ?$

$\text{tr} \begin{bmatrix} -1 & \phantom{1} \\ 1 & \phantom{1} \end{bmatrix} = ?$

drawing: M.M. Julian
Foundations of Crystallography
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Description of isometries

Coordinate system: \{O, a, b, c\}

Isometry:

\[ \tilde{x} = F_1(x, y, z) \]

\[ \tilde{x} = W_{11} x + W_{12} y + W_{13} z + w_1 \]
\[ \tilde{y} = W_{21} x + W_{22} y + W_{23} z + w_2 \]
\[ \tilde{z} = W_{31} x + W_{32} y + W_{33} z + w_3 \]
Matrix-column presentation of isometries

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

linear/matrix part

\[
\tilde{x} = W x + w
\]

matrix-column pair

\[
\tilde{x} = (W, w) x \quad \text{or} \quad \tilde{x} = \{W | w\} x
\]

Seitz symbol
Referred to an ‘orthorhombic’ coordinated system \((a \neq b \neq c; \alpha = \beta = \gamma = 90)\) two symmetry operations are represented by the following matrix-column pairs:

\[
(W_1, w_1) = \begin{pmatrix}
-1 & 0 \\
0 & 1 \\
-1 & 0
\end{pmatrix} \quad (W_2, w_2) = \begin{pmatrix}
-1 & 1/2 \\
0 & 0 \\
-1 & 1/2
\end{pmatrix}
\]

Determine the images \(X_i\) of a point \(X\) under the symmetry operations \((W_i, w_i)\) where \(X = \begin{pmatrix} 0.70 \\
0.31 \\
0.95 \end{pmatrix}\)

Can you guess what is the geometric ‘nature’ of \((W_1, w_1)\)?

And of \((W_2, w_2)\)?

\textit{Hint:}\n
A drawing could be rather helpful.
Characterization of the symmetry operations:

\[
\begin{vmatrix}
-1 & 1 & -1 \\
1 & -1 & 1 \\
-1 & 1 & -1 \\
\end{vmatrix}
\]
\[= \ ?\]

\[
\begin{vmatrix}
-1 & 1 & -1 \\
1 & -1 & 1 \\
-1 & 1 & -1 \\
\end{vmatrix}
\]
\[= \ ?\]

What are the fixed points of \((W_1,w_1)\) and \((W_2,w_2)\) ?
Short-hand notation for the description of isometries

**isometry:**

\[
\begin{align*}
\tilde{x} &= W_{11} x + W_{12} y + W_{13} z + w_1 \\
\tilde{y} &= W_{21} x + W_{22} y + W_{23} z + w_2 \\
\tilde{z} &= W_{31} x + W_{32} y + W_{33} z + w_3,
\end{align*}
\]

**notation rules:**
- left-hand side: omitted
- coefficients 0, +1, -1
- different rows in one line

**examples:**

\[
\begin{array}{c|c|c|c}
-1 & 1/2 & \\
1 & 0 & \\
-1 & 1/2 & \\
\end{array}
\rightarrow \{ -x+1/2, y, -z+1/2 \}

\begin{array}{c|c|c|c}
1 & 0 & \\
0 & 1 & \\
-1 & 1/2 & \\
\end{array}
\rightarrow \{ x+1/2, y, z+1/2 \}
Construct the matrix-column pair \((W,w)\) of the following coordinate triplets:

(1) \(x,y,z\)  
(2) \(-x,y+1/2,-z+1/2\)  
(3) \(-x,-y,-z\)  
(4) \(x,-y+1/2, z+1/2\)
\[ \tilde{x} = Ux + u; \]
\[ \tilde{x} = V\tilde{x} + v; \]
\[ \tilde{x} = V(Ux + u) + v; \]
\[ \tilde{x} = VUx + Vu + v = Wx + w. \]

\[ \tilde{x} = (V, v)\tilde{x} = (V, v)(U, u)x = (W, w)x. \]

\[ (W, w) = (V, v)(U, u) = (VU, Vu + v). \]
Consider the matrix-column pairs of the two symmetry operations:

\[
(W_1, w_1) = \begin{pmatrix}
0 & -1 & 0 \\
1 & 0 & 0 \\
0 & 1 & 0
\end{pmatrix}
\quad \text{and} \quad
(W_2, w_2) = \begin{pmatrix}
-1 & 0 & 1/2 \\
0 & 1 & 0 \\
1 & -1 & 1/2
\end{pmatrix}
\]

Determine and compare the matrix-column pairs of the combined symmetry operations:

\[
(W, w) = (W_1, w_1)(W_2, w_2)
\]

\[
(W, w)' = (W_2, w_2)(W_1, w_1)
\]

combination of isometries:

\[
(W_2, w_2)(W_1, w_1) = (W_2 W_1, W_2 w_1 + w_2)
\]
Inverse isometries

\[ X \xrightarrow{(W,w)} \tilde{X} \]

\[ X \approx (C,c) = (W,w)^{-1} \]

\[ (C,c)(W,w) = (I,o) \quad I = 3\times3 \text{ identity matrix} \]

\[ (C,c)(W,w) = (CW, Cw + c) \]

\[ CW = I \]

\[ C = W^{-1} \]

\[ Cw + c = o \]

\[ c = -Cw = -W^{-1}w \]
Determine the inverse symmetry operations \((W_1, w_1)^{-1}\) and \((W_2, w_2)^{-1}\) where

\[
(W_1, w_1) = \begin{pmatrix}
0 & -1 & 0 \\
1 & 0 & 0 \\
0 & 1 & 0
\end{pmatrix} \quad (W_2, w_2) = \begin{pmatrix}
-1 & 1/2 \\
1 & 0 \\
-1 & 1/2
\end{pmatrix}
\]

Determine the inverse symmetry operation \((W, w)^{-1}\)

\[(W, w) = (W_1, w_1)(W_2, w_2)\]

inverse of isometries:

\[(W, w)^{-1} = (W^{-1}, -W^{-1}w)\]
Consider the matrix-column pairs

\[(A, a) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} \quad \text{and} \quad (B, b) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}\]

(i) What is the matrix-column pair resulting from \((B, b)(A, a) = (C, c)\), and \((A, a)(B, b) = (D, d)\) ?

(ii) What is \((A, a)^{-1}\), \((B, b)^{-1}\), \((C, c)^{-1}\) and \((D, d)^{-1}\) ?

(iii) What is \((B, b)^{-1}(A, a)^{-1}\) ?
Matrix formalism: $4\times 4$ matrices

\[ x \rightarrow \tilde{x} = \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}; \quad \tilde{x} \rightarrow \tilde{x} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ 1 \end{pmatrix} \]

augmented matrices:

\[ (W, w) \rightarrow \tilde{W} = \begin{pmatrix} W & w \\ 0 & 0 & 0 & 1 \end{pmatrix} \]

point $X \rightarrow$ point $\tilde{X}$:

\[ \tilde{x} = \tilde{W} x \]

\[ \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ 1 \end{pmatrix} = \begin{pmatrix} W & w \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} \]
4x4 matrices: general formulae

Point $X \rightarrow$ point $\tilde{X}$:

\[
\begin{pmatrix}
\tilde{x} \\
\tilde{y} \\
\tilde{z} \\
1
\end{pmatrix} = \begin{pmatrix}
W & w \\
0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z \\
1
\end{pmatrix}
\]

Combination and inverse of isometries:

\[
(W)^{-1} = (W^{-1})
\]
\[
W^{-1} = \begin{pmatrix}
W^{-1} & -W^{-1}w \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

$W_3 = W_2 W_1$
Construct the (4x4) matrix-presentation of the following coordinate triplets:

(1) \(x, y, z\)  
(2) \(-x, y + 1/2, -z + 1/2\)  
(3) \(-x, -y, -z\)  
(4) \(x, -y + 1/2, z + 1/2\)
**Crystallographic symmetry operations**

**Symmetry operations of an object**

The isometries which map the object onto itself are called *symmetry operations of this object*. The *symmetry* of the object is the set of all its symmetry operations.

**Crystallographic symmetry operations**

If the object is a crystal pattern, representing a real crystal, its symmetry operations are called *crystallographic symmetry operations*.

The equilateral triangle allows six symmetry operations: rotations by 120° and 240° around its centre, reflections through the three thick lines intersecting the centre, and the identity operation.
Crystallographic symmetry operations

characteristics: fixed points of isometries \((W, w)X_f = X_f\) geometric elements

Types of isometries preserve handedness

identity: the whole space fixed

translation \(t\): no fixed point \(\tilde{x} = x + t\)

rotation: one line fixed rotation axis \(\phi = k \times \frac{360^\circ}{N}\)

screw rotation: no fixed point screw axis screw vector
Rotation (around an axis)

Rotation of order $n = \text{rotation by } \varphi = \frac{2\pi}{n}$

$$\alpha(n) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{Det} = +1$$
Crystallographic symmetry operations

**Screw rotation**

$n$-fold rotation followed by a fractional translation $\frac{p}{n} \mathbf{t}$ parallel to the rotation axis.

Its application $n$ times results in a translation parallel to the rotation axis.
<table>
<thead>
<tr>
<th>Types of isometries</th>
<th>do not preserve handedness</th>
</tr>
</thead>
<tbody>
<tr>
<td>roto-inversion:</td>
<td>centre of roto-inversion fixed</td>
</tr>
<tr>
<td></td>
<td>roto-inversion axis</td>
</tr>
<tr>
<td>inversion:</td>
<td>centre of inversion fixed</td>
</tr>
<tr>
<td>reflection:</td>
<td>plane fixed</td>
</tr>
<tr>
<td></td>
<td>reflection/mirror plane</td>
</tr>
<tr>
<td>glide reflection:</td>
<td>no fixed point</td>
</tr>
<tr>
<td></td>
<td>glide plane</td>
</tr>
<tr>
<td></td>
<td>glide vector</td>
</tr>
</tbody>
</table>
Symmetry operations in 3D
Rotoinvertions

**Inversion (through a point)**

A crystal which has the inversion symmetry is called **centrosymmetrical**.

\[
\alpha(\bar{1}) = \begin{pmatrix}
-1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & -1 \\
\end{pmatrix}
\]

\[\text{Det} = -1\]
Symmetry operations in 3D
Rotoinversions

**Roto-inversion**
(around an axis and through a point)

*Rotation followed by an inversion*

$$
\alpha(\vec{n}) = \begin{pmatrix}
-\cos \phi & \sin \phi & 0 \\
-\sin \phi & -\cos \phi & 0 \\
0 & 0 & -1
\end{pmatrix}
\quad \text{Det} = -1
$$
Symmetry operations in 3D
Rotoinvertions

Reflection (through a mirror plane)

Note that: $m = 2$

$\alpha(\bar{1}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

$\text{Det} = -1$
Crystallographic symmetry operations

Glide plane

reflection followed by a fractional translation \( \frac{1}{2} \mathbf{t} \) parallel to the plane

Its application 2 times results in a translation parallel to the plane
Matrix-column presentation of some symmetry operations

Rotation or roto-inversion around the origin:

\[
\begin{pmatrix}
  w & w & w & 0 \\
  w & w & w & 0 \\
  w & w & w & 0
\end{pmatrix}
\begin{pmatrix}
  x \\
  y \\
  z
\end{pmatrix}
= 
\begin{pmatrix}
  0 \\
  0 \\
  0
\end{pmatrix}
\]

Translation:

\[
\begin{pmatrix}
  1 & w1 \\
  1 & w2 \\
  1 & w3
\end{pmatrix}
\begin{pmatrix}
  x \\
  y \\
  z
\end{pmatrix}
= 
\begin{pmatrix}
  x+w1 \\
  y+w2 \\
  z+w3
\end{pmatrix}
\]

Inversion through the origin:

\[
\begin{pmatrix}
  -1 & 0 & 0 \\
  -1 & 0 & 0 \\
  -1 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
  x \\
  y \\
  z
\end{pmatrix}
= 
\begin{pmatrix}
  -x \\
  -y \\
  -z
\end{pmatrix}
\]
**Geometric meaning of** \((W, w)\) **information**

(a) type of isometry

<table>
<thead>
<tr>
<th>(\text{tr}(W))</th>
<th>(\det(W) = +1)</th>
<th>(\det(W) = -1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 2 1 0 -1</td>
<td>-3 -2 -1 0 1</td>
<td></td>
</tr>
<tr>
<td>type</td>
<td>1 6 4 3 2</td>
<td>1 6 4 3 2</td>
</tr>
<tr>
<td>order</td>
<td>1 6 4 3 2</td>
<td>2 6 4 6 2</td>
</tr>
</tbody>
</table>

**order:** \(W^n = I\)

**rotation angle**

\[
\cos \varphi = \frac{\pm \text{tr}(W) - 1}{2}
\]
Determine the type and order of isometries that are represented by the following matrix-column pairs:

(1) \( x, y, z \)  
(2) \(-x, y + 1/2, -z + 1/2\)  
(3) \(-x, -y, -z\)  
(4) \(x, -y + 1/2, z + 1/2\)

(a) type of isometry

<table>
<thead>
<tr>
<th>( \text{tr}(W) )</th>
<th>( \text{det}(W) = +1 )</th>
<th>( \text{det}(W) = -1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 3 )</td>
<td>( 2 )</td>
<td>( -3 )</td>
</tr>
<tr>
<td>( 2 )</td>
<td>( 1 )</td>
<td>( -2 )</td>
</tr>
<tr>
<td>( 1 )</td>
<td>( 0 )</td>
<td>( -1 )</td>
</tr>
<tr>
<td>( 0 )</td>
<td>( -1 )</td>
<td>( 0 )</td>
</tr>
<tr>
<td>( -1 )</td>
<td>( 1 )</td>
<td>( 1 )</td>
</tr>
</tbody>
</table>

| type | \( 1 \) | \( 6 \) | \( 4 \) | \( 3 \) | \( 2 \) | \( \overline{1} \) | \( \overline{6} \) | \( \overline{4} \) | \( \overline{3} \) | \( \overline{2} = m \) |
| order| \( 1 \) | \( 6 \) | \( 4 \) | \( 3 \) | \( 2 \) | \( 2 \) | \( 6 \) | \( 4 \) | \( 6 \) | \( 2 \) |
Consider the matrix-column pairs

\[
(A, a) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}
\]
and

\[
(B, b) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}
\]

(i) What is the matrix-column pair resulting from \((B, b)(A, a) = (C, c)\), and \((A, a)(B, b) = (D, d)\)?
(ii) What is \((A, a)^{-1}\), \((B, b)^{-1}\), \((C, c)^{-1}\) and \((D, d)^{-1}\)?
(iii) What is \((B, b)^{-1}(A, a)^{-1}\)?

Determine the type and order of isometries that are represented by the matrices \(A, B, C\) and \(D\):
Geometric meaning of $(W, w)$ information

(b) axis or normal direction $u$:
\[ Wu = \pm u \]

(b1) rotations:
\[ Y(W) = W^{k-1} + W^{k-2} + \ldots + W + I \]

(b2) roto-inversions:
\[ Y(-W) = -W + I \]

reflections:
Direction of rotation axis/normal

Example: $(W, w) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$det W = ?$
$tr W = ?$

What is the type and order of the isometry?
Determine its rotation axis?

$Y(W) = W^{k-1} + W^{k-2} + \ldots + W + I$

$Y(W) =$

$W^3$ + $W^2$ + $W$ + $I$ =

$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}$
Determine the rotation or rotoinversion axes (or normals in case of reflections) of the following symmetry operations

(2) \(-x, y+1/2, -z+1/2\)  \hspace{1cm} (4) \(x, -y+1/2, z+1/2\)

rotations: \[ Y(W) = W^{k-1} + W^{k-2} + \ldots + W + I \]

reflections: \[ Y(-W) = -W + I \]
Geometric meaning of $(W, w)$ information

(c) sense of rotation:

for rotations or rotoinversions with $k>2$

$$\det(Z): \ Z = [u | x | (\det W) \ W x]$$

$x$ non-parallel to $u$
Sense of rotation

Example: 

$$(W,w) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$\det W = 1$ \hspace{1cm} $\text{tr} \ W = 1$

$W = 4_{001}$

What is its sense of rotation?

$\det(Z): \quad Z = [u | x | (\det W) \ W x]$
Fixed points of isometries

\[(W, w)X_f = X_f\]

\[
\begin{pmatrix}
  -1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 0 \\
  0 & 0 & -1 & 1/2 \\
\end{pmatrix}
\begin{pmatrix}
  x \\
  y \\
  z \\
\end{pmatrix} =
\begin{pmatrix}
  x \\
  y \\
  z \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
  -1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 1/2 \\
  0 & 0 & -1 & 1/2 \\
\end{pmatrix}
\begin{pmatrix}
  x \\
  y \\
  z \\
\end{pmatrix} =
\begin{pmatrix}
  x \\
  y \\
  z \\
\end{pmatrix}
\]

Fixed points?

Translation part \( w = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} \)

Intrinsic (screw, glide) location
Glide or Screw component (intrinsic translation part)

\[(W, w)^k = (W, w) \cdot (W, w) \cdot \ldots \cdot (W, w) = (I, t)\]

\[(W, w)^k = (W^k, (W^{k-1} + \ldots + W + I)w) = (I, t)\]

screw rotations: \[
\frac{t}{k} = \frac{1}{k} \cdot \frac{I}{k} (W^{k-1} + \ldots + W + I)w
\]

glide reflections: \[
\frac{t}{k} = \frac{1}{2} (W + I)w
\]
Determine the intrinsic translation parts (if relevant) of the following symmetry operations:

(1) \( x, y, z \)  
(2) \( -x, y + 1/2, -z + 1/2 \)  
(3) \( -x, -y, -z \)  
(4) \( x, -y + 1/2, z + 1/2 \)

**Screw Rotations:**
\[ t/k = l/k (W^{k-1} + \ldots + W + I)w \]

**Glide Reflections:**
\[ t/k = \frac{1}{2} (W + I)w \]
Fixed points of \((W,w)\):

Location (fixed points \(x_F\)):

\[(B1) \ t/k = 0:\]
\[
(W, w)x_F = x_F
\]

\[(B2) \ t/k \neq 0:\]
\[
(W, w_{lp})x_F = x_F
\]
\[
w_{lp} = w - t/k
\]
Determine the fixed points of the following symmetry operations:

(1) \(x, y, z\)  
(2) \(-x, y + 1/2, -z + 1/2\)  
(3) \(-x, -y, -z\)  
(4) \(x, -y + 1/2, z + 1/2\)

fixed points: \(\mathbf{W}, \mathbf{w}_{lp}\)x_F = x_F\)
Space group $P2_1/c$ (No. 14)

**No. 14**

$P12_1/c1$

**UNIQUE AXIS $b$, CELL CHOICE 1**

**EXAMPLE**

**Generators selected**

$(1); t(1,0,0); t(0,1,0); t(0,0,1); (2); (3)$

**Positions**

Multiplicity, Wyckoff letter, Site symmetry

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Site symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>$e$</td>
<td>1</td>
</tr>
</tbody>
</table>

**Coordinates**

1. $(x,y,z)$
2. $x, y + \frac{1}{2}, z + \frac{1}{2}$
3. $x, y, z$
4. $x, y + \frac{1}{2}, z + \frac{1}{2}$

**Matrix-column presentation**

**Geometric interpretation**

\[
\tilde{x} = Ux + u;
\]

\[
\tilde{x} = Vx + v;
\]

\[
\tilde{x} = V(Ux + u) + v;
\]

\[
\tilde{x} = Wx + w.
\]
Crystallographic databases

- Group-subgroup relations
- Structural utilities
- Representations of point and space groups
- Solid-state applications
Crystallographic Databases

International Tables for Crystallography
Construct the matrix-column pairs \((W,w)\) of the following coordinate triplets:

1. \((x, y, z)\)
2. \((-x, y+\frac{1}{2}, -z+\frac{1}{2})\)
3. \((-x, -y, -z)\)
4. \((x, -y+\frac{1}{2}, z+\frac{1}{2})\)

Characterize geometrically these matrix-column pairs taking into account that they refer to a monoclinic basis with unique axis \(b\).

Use the program SYMMETRY OPERATIONS for the geometric interpretation of the matrix-column pairs of the symmetry operations.
Problem: Geometric Interpretation of (W,w)

Symmetry Operation

This program calculates the geometric interpretation of matrix column representation of symmetry operation for a given crystal system or space group.

Input:

i) The crystal system or the space group number.

ii) The matrix column representation of symmetry operation.

If you want to work on a non conventional setting click on Non conventional setting, this will show you a form where you have to introduce the transformation matrix relating the conventional setting of the group you have chosen with the non conventional one you are interested in.

Output:

We obtain the geometric interpretation of the symmetry operation.

-\( x, y + 1/2, -z + 1/2 \)

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

\( (0, 1/2, 0), 0, y, 1/4 \)
COORDINATE TRANSFORMATIONS IN CRYSTALLOGRAPHY
Co-ordinate transformation

3-dimensional space

\((a, b, c), \text{ origin } O: \text{ point } X(x, y, z)\)

\((p, \rho) \downarrow\)

\((a', b', c'), \text{ origin } O': \text{ point } X(x', y', z')\)

Transformation matrix-column pair \((p, \rho)\)

(i) linear part: change of orientation or length:

\[
(a', b', c') = (a, b, c)P
\]

\[
= (a, b, c) \begin{pmatrix}
P_{11} & P_{12} & P_{13} \\
P_{21} & P_{22} & P_{23} \\
P_{31} & P_{32} & P_{33}
\end{pmatrix} = (P_{11}a + P_{21}b + P_{31}c, P_{12}a + P_{22}b + P_{32}c, P_{13}a + P_{23}b + P_{33}c).
\]

(ii) origin shift by a shift vector \(p(p_1, p_2, p_3)\):

\[
O' = O + p
\]

the origin \(O'\) has coordinates \((p_1, p_2, p_3)\) in the old coordinate system
Write “new in terms of old” as column vectors.

\[ (a', b', c') = (a, b, c) \]

\[ (a, b, c) = (a', b', c') \]

\[ X = \left( \frac{3}{4}, \frac{1}{4}, 0 \right) \]

\[ X' = \left( \text{?} \right) \]
Linear parts as before.
Transformation matrix-column pair \((P,p)\)

\[
(P,p) = \begin{pmatrix}
\frac{1}{2} & \frac{1}{2} & 0 \\
-\frac{1}{2} & \frac{1}{2} & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

\[
(P,p)^{-1} = \begin{pmatrix}
1 & -1 & 0 \\
1 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

\[
a' = \frac{1}{2}a - \frac{1}{2}b \\
b' = \frac{1}{2}a + \frac{1}{2}b \\
c' = c
\]

\[
O' = O + \begin{pmatrix}
\frac{1}{2} \\
\frac{1}{4} \\
0
\end{pmatrix}
\]

\[
a = a' + b' \\
b = -a' + b' \\
c = c' \\
O = O' + \begin{pmatrix}
-\frac{1}{4} \\
-\frac{3}{4} \\
0
\end{pmatrix}
\]
Transformation of the coordinates of a point \( X(x,y,z) \):

\[
(X') = ((P,p)^{-1}(X) = (P^{-1}, -P^{-1}p)(X)
\]

special cases

- origin shift \((P=I)\):
  \[
x' = x - p
\]

- change of basis \((p=o)\):
  \[
x' = P^{-1}x
\]

Transformation of symmetry operations \((W,w)\):

\[
(W',w') = ((P,p)^{-1}(W,w)(P,p)
\]

Transformation by \((P,p)\) of the unit cell parameters:

metric tensor \(G\):

\[
G' = P^t \cdot G \cdot P
\]
Short-hand notation for the description of transformation matrices

**Transformation matrix:**

\[
\begin{pmatrix}
P & P & P & p_1 \\
P & P & P & p_2 \\
P & P & P & p_3 \\
P & P & P & p_4 \\
\end{pmatrix}
\]

\((a',b',c'),\text{ origin } O'\)

\((a,b,c),\text{ origin } O\)

**notation rules:**
- written by **columns**
- coefficients 0, +1, -1
- different **columns** in one line
- origin shift

**example:**

\[
\begin{pmatrix}
1 & -1 & -1/4 \\
1 & 1 & -3/4 \\
0 & 0 & 0 \\
\end{pmatrix}
\]

\(\{a+b, -a+b, c; -1/4, -3/4, 0\}\)
The following matrix-column pairs \((W,w)\) are referred with respect to a basis \((a,b,c)\):

1. \(x, y, z\)
2. \(-x, y + 1/2, -z + 1/2\)
3. \(-x, -y, -z\)
4. \(x, -y + 1/2, z + 1/2\)

Determine the corresponding matrix-column pairs \((W',w')\) with respect to the basis \((a',b',c') = (a,b,c)P\), with \(P = c, a, b\).

Determine the coordinates \(X'\) of a point \(X = \begin{bmatrix} 0.70 \\ 0.31 \\ 0.95 \end{bmatrix}\) with respect to the new basis \((a',b',c')\).