Definitions and conventions

Information in this page is valid for spglib 1.8.1 or later. The definitions of transformation matrix and origin shift were different in the previous versions.

- Basis vectors $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ or $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$
- Atomic point coordinates $\boldsymbol{x}$
- Symmetry operation $(\boldsymbol{W}, \boldsymbol{w})$
- Transformation matrix $\boldsymbol{P}$ and origin shift $\boldsymbol{p}$
- Conventions of standardized unit cell
  - Choice of basis vectors
  - Transformation to the primitive cell
  - Idealization of unit cell structure

Basis vectors $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ or $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$

In spglib, basis vectors are represented by three column vectors:

$$\mathbf{a} = \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix}, \mathbf{b} = \begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix}, \mathbf{c} = \begin{pmatrix} c_x \\ c_y \\ c_z \end{pmatrix},$$

in Cartesian coordinates. Depending on the situation, $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ is used instead of $(\mathbf{a}, \mathbf{b}, \mathbf{c})$.

Atomic point coordinates $\boldsymbol{x}$

Coordinates of an atomic point $\boldsymbol{x}$ are represented as three fractional values relative to basis vectors as follows,

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix},$$

where $0 \leq x_i < 1$. A position vector $\mathbf{x}$ in Cartesian coordinates is obtained by

$$\mathbf{x} = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{x}.$$

or

$$\mathbf{x} = \sum_i x_i \mathbf{a}_i.$$

Symmetry operation $(\boldsymbol{W}, \boldsymbol{w})$

A symmetry operation consists of a pair of the rotation part $\boldsymbol{W}$ and translation part $\boldsymbol{w}$, and is represented as $(\boldsymbol{W}, \boldsymbol{w})$ in the spglib document. The symmetry operation transfe $\tilde{\boldsymbol{x}}$ as follows:

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}.$$

Transformation matrix $\boldsymbol{P}$ and origin shift $\boldsymbol{p}$

The transformation matrix $\boldsymbol{P}$ changes choice of basis vectors as follows

$$(\mathbf{a}\ \mathbf{b}\ \mathbf{c}) = (\mathbf{a}_\mathrm{s}\ \mathbf{b}_\mathrm{s}\ \mathbf{c}_\mathrm{s})\boldsymbol{P},$$

where $(\mathbf{a}\ \mathbf{b}\ \mathbf{c})$ and $(\mathbf{a}_\mathrm{s}\ \mathbf{b}_\mathrm{s}\ \mathbf{c}_\mathrm{s})$ are the basis vectors of an arbitrary system and of a starndardized system, respectively. Transformation matrix **doesn't** rotate a crystal in Cartesi coordinates, but just changes the choices of basis vectors.

The origin shift $\boldsymbol{p}$ gives the vector from the origin of the standardized system $\boldsymbol{O}_\mathrm{s}$ to the origin of the arbitrary system $\boldsymbol{O}$,

$$\boldsymbol{p} = \boldsymbol{O} - \boldsymbol{O}_\mathrm{s}.$$

Origin shift **doesn't** move a crystal in Cartesian coordinates, but just changes the origin to measure the coordinates of atomic points.

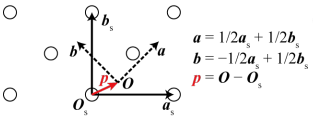
A change of basis is described by the combination of the transformation matrix and the origin shift denoted by $(\boldsymbol{P}, \boldsymbol{p})$ where first the transformation matrix is applied and then shift. The points in the standardized system $\boldsymbol{x}_\mathrm{s}$ and arbitrary system $\boldsymbol{x}$ are related by

$$\boldsymbol{x}_\mathrm{s} = \boldsymbol{P}\boldsymbol{x} + \boldsymbol{p},$$

or equivalently,

$$\boldsymbol{x} = \boldsymbol{P}^{-1}\boldsymbol{x}_\mathrm{s} - \boldsymbol{P}^{-1}\boldsymbol{p}.$$

A graphical example is shown below.



(_images/change-of-basis.png)

(click the figure to enlarge)

In this example,

$$\boldsymbol{P} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{\frac{1}{2}} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Conventions of standardized unit cell

Choice of basis vectors

Using the APIs `spg_get_dataset` , `spg_get_dataset_with_hall_number` , or `spg_standardize_cell` , the starndardized unit cell is obtained. The “starndardized un cell” in this document means that the (conventional) unit cell structure is standardized by the crystal symmetry and lengths of basis vectors. Crystals are categorized by Hall sym in 530 different types in terms of 230 space group types, unique axes, settings, and cell choices. Moreover in spglib, lengths of basis vectors are used to choose the order of $(\mathbf{a}, \mathbf{b},$ the order can not be determined only by the symmetrical conventions. The details of these conventions are summarized in the article found at http://arxiv.org/abs/1506.01455 (http://arxiv.org/abs/1506.01455).

Transformation to the primitive cell

In the standardized unit cells, there are five different centring types available, base centrings of A and C, rhombohedral (R), body centred (I), and face centred (F). The transforma applied to the standardized unit cell by

$$(\mathbf{a}_\mathrm{p}\ \mathbf{b}_\mathrm{p}\ \mathbf{c}_\mathrm{p}) = (\mathbf{a}_\mathrm{s}\ \mathbf{b}_\mathrm{s}\ \mathbf{c}_\mathrm{s})\boldsymbol{P}_\mathrm{c},$$

where $\mathbf{a}_\mathrm{p}$, $\mathbf{b}_\mathrm{p}$, and $\mathbf{c}_\mathrm{p}$ are the basis vectors of the primitive cell and $\boldsymbol{P}_\mathrm{c}$ is the transformation matrix from the standardized unit cell to the primitive cell. $\boldsymbol{P}_\mathrm{c}$ for centring types are as follows:

$$\boldsymbol{P}_\mathrm{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & \bar{\frac{1}{2}} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}, \boldsymbol{P}_\mathrm{C} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{\frac{1}{2}} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \boldsymbol{P}_\mathrm{R} = \begin{pmatrix} \frac{2}{3} & \bar{\frac{1}{3}} & \bar{\frac{1}{3}} \\ \frac{1}{3} & \frac{1}{3} & \bar{\frac{2}{3}} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}, \boldsymbol{P}_\mathrm{I} = \begin{pmatrix} \bar{\frac{1}{2}} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \bar{\frac{1}{2}} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \bar{\frac{1}{2}} \end{pmatrix}, \boldsymbol{P}_\mathrm{F} = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}.$$

For rhombohedral lattice systems with the choice of hexagonal axes, $\boldsymbol{P}_\mathrm{R}$ is applied.

Idealization of unit cell structure

Spglib allows tolerance parameters to match a slightly distorted unit cell structure to a space group type with some higher symmetry. Using obtained symmetry operations, the distortion is removed to idealize the unit cell structure. The coordinates of atomic points are idealized using respective site-symmetries (Grosse-Kunstleve *et al.* (2002)). The basis vectors are idealized by forceing them into respective lattice shapes as follows. In this treatment, except for triclinic crystals, crystals can be rotated in Cartesian coordinates, whi the different type of transformation from that of the change-of-basis transformation explained above.

Triclinic lattice

- Niggli reduced cell is used for choosing $\mathbf{a}, \mathbf{b}, \mathbf{c}$.
- $\mathbf{a}$ is set along $+x$ direction of Cartesian coordinates.
- $\mathbf{b}$ is set in x-y plane of Cartesian coordinates so that $\mathbf{a} \times \mathbf{b}$ is along $+z$ direction of Cartesian coordinates.

Monoclinic lattice

- b axis is taken as the unique axis.
- $\alpha = 90°$ and $\gamma = 90°$
- $90° < \beta < 120°$.
- $\mathbf{a}$ is set along $+x$ direction of Cartesian coordinates.
- $\mathbf{b}$ is set along $+y$ direction of Cartesian coordinates.
- $\mathbf{c}$ is set in x-z plane of Cartesian coordinates.

Orthorhombic lattice

- $\alpha = \beta = \gamma = 90°$.
- $\mathbf{a}$ is set along $+x$ direction of Cartesian coordinates.
- $\mathbf{b}$ is set along $+y$ direction of Cartesian coordinates.
- $\mathbf{c}$ is set along $+z$ direction of Cartesian coordinates.

Tetragonal lattice

- $\alpha = \beta = \gamma = 90°$.
- $a = b$.
- $\mathbf{a}$ is set along $+x$ direction of Cartesian coordinates.
- $\mathbf{b}$ is set along $+y$ direction of Cartesian coordinates.
- $\mathbf{c}$ is set along $+z$ direction of Cartesian coordinates.

Rhombohedral lattice

- $\alpha = \beta = \gamma$.
- $a = b = c$.
- Let $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ projected on x-y plane in Cartesian coordinates be $\mathbf{a}_{xy}$, $\mathbf{b}_{xy}$, and $\mathbf{c}_{xy}$, respectively, and their angles be α_{xy}, β_{xy}, γ_{xy}, respectively.
- Let $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ projected along z-axis in Cartesian coordinates be $\mathbf{a}_z$, $\mathbf{b}_z$, and $\mathbf{c}_z$, respectively.
- $\mathbf{a}_{xy}$ is set along $+x$ direction of Cartesian coordinates, and $\mathbf{b}_{xy}$ and $\mathbf{c}_{xy}$ are placed by angles 120° and 240° from $\mathbf{a}_{xy}$ counter-clockwise, respectively.
- $\alpha_{xy} = \beta_{xy} = \gamma_{xy} = 120^\circ$.
- $a_{xy} = b_{xy} = c_{xy}$.
- $a_z = b_z = c_z$.

Hexagonal lattice

- $\alpha = \beta = 90^\circ$.
- $\gamma = 120^\circ$.
- $a = b$.
- $\mathbf{a}$ is set along $+x$ direction of Cartesian coordinates.
- $\mathbf{b}$ is set in x-y plane of Cartesian coordinates.
- $\mathbf{c}$ is set along $+z$ direction of Cartesian coordinates.

Cubic lattice

- $\alpha = \beta = \gamma = 90^\circ$.
- $a = b = c$.
- $\mathbf{a}$ is set along $+x$ direction of Cartesian coordinates.
- $\mathbf{b}$ is set along $+y$ direction of Cartesian coordinates.
- $\mathbf{c}$ is set along $+z$ direction of Cartesian coordinates.
