$\mathbf{e}_x \parallel \mathbf{a}$, $\mathbf{e}_y \parallel (\mathbf{c}^* \times \mathbf{a})$, $\mathbf{e}_z \parallel \mathbf{c}^*$ **default PDB convention**

Definitions

a, **b**, **c** - *cell axes, cristallographic basis*

a, b, c - cell size

α, β, γ - *cell angles*

$\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ - *orthonormal basis*

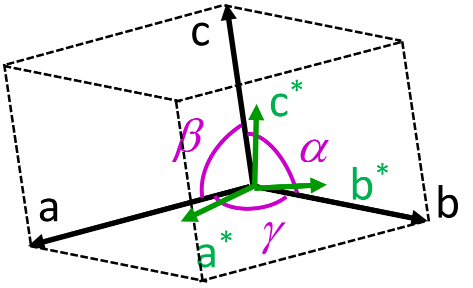
$\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ - *conjugate basis*

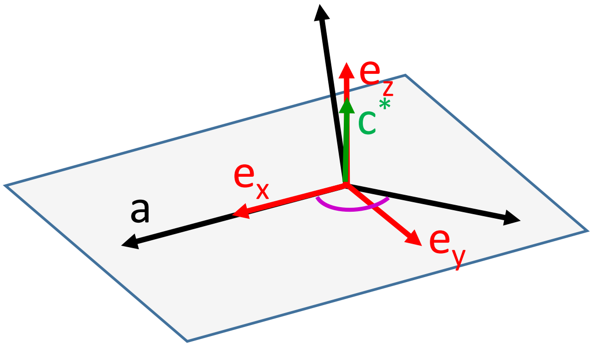
$\cos\alpha^* =$

$= (\cos\beta\cdot\cos\gamma - \cos\alpha) / (\sin\beta\cdot\sin\gamma)$

$\cos\beta^* =$

$= (\cos\gamma\cdot\cos\alpha - \cos\beta) / (\sin\gamma\cdot\sin\alpha)$





Orthogonalisation matrix :

$$\begin{pmatrix} a & b\cdot\cos\gamma & c\cdot\cos\beta \\ 0 & b\cdot\sin\gamma & -c\cdot\cos\alpha^*\cdot\sin\beta \\ 0 & 0 & c\cdot\sin\alpha^*\cdot\sin\beta \end{pmatrix}$$

Deorthogonalisation matrix :

$$\begin{pmatrix} 1/a & -1/(a\cdot\tan\gamma) & \sin\alpha\cdot\cos\beta^*/(a\cdot\sin\alpha^*\cdot\sin\beta\cdot\sin\gamma) \\ 0 & 1/(b\cdot\sin\gamma) & 1/(b\cdot\tan\alpha^*\cdot\sin\gamma) \\ 0 & 0 & 1/(c\cdot\sin\alpha^*\cdot\sin\beta) \end{pmatrix}$$

$e_x \parallel b$, $e_y \parallel (a^* \times b)$, $e_z \parallel a^*$

Definitions

a, **b**, **c** - *cell axes, cristallographic basis*

a, b, c - cell size

α, β, γ - *cell angles*

$\mathbf{e_x}$, $\mathbf{e_y}$, $\mathbf{e_z}$ - *orthonormal basis*

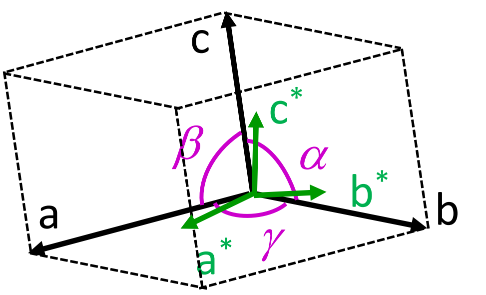
$\mathbf{a^*}$, $\mathbf{b^*}$, $\mathbf{c^*}$ - *conjugate basis*

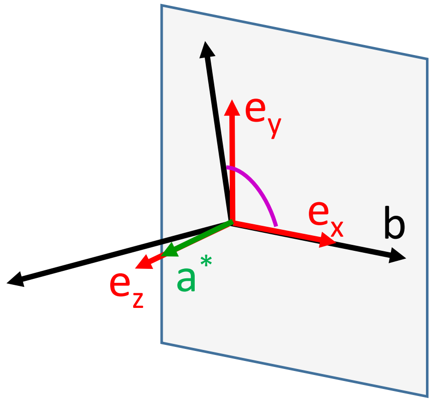
$\cos\beta^* =$

$= (\cos\gamma \cdot \cos\alpha - \cos\beta) / (\sin\gamma \cdot \sin\alpha)$

$\cos\gamma^* =$

$= (\cos\alpha \cdot \cos\beta - \cos\gamma) / (\sin\alpha \cdot \sin\beta)$





Orthogonalisation matrix :

$$\begin{pmatrix} a \cdot \cos\gamma & b & c \cdot \cos\alpha \\ -a \cdot \cos\beta^* \cdot \sin\gamma & 0 & c \cdot \sin\alpha \\ a \cdot \sin\beta^* \cdot \sin\gamma & 0 & 0 \end{pmatrix}$$

Deorthogonalisation matrix :

$$\begin{pmatrix} 0 & 0 & 1/(a \cdot \sin\beta^* \cdot \sin\gamma) \\ 1/b & -1/(b \cdot \tan\alpha) & \sin\beta \cdot \cos\gamma^* / (b \cdot \sin\alpha \cdot \sin\beta^* \cdot \sin\gamma) \\ 0 & 1/(c \cdot \sin\gamma) & 1/(c \cdot \sin\alpha \cdot \tan\beta^*) \end{pmatrix}$$

$\mathbf{e}_x \parallel \mathbf{c}$, $\mathbf{e}_y \parallel (\mathbf{b}^* \times \mathbf{c})$, $\mathbf{e}_z \parallel \mathbf{b}^*$

Definitions

a, **b**, **c** - *cell axes, cristallographic basis*

a, b, c - cell size

α, β, γ - *cell angles*

$\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ - *orthonormal basis*

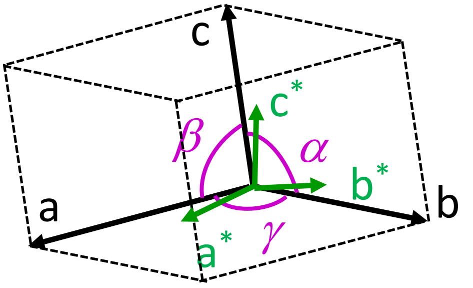
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ - *conjugate basis*

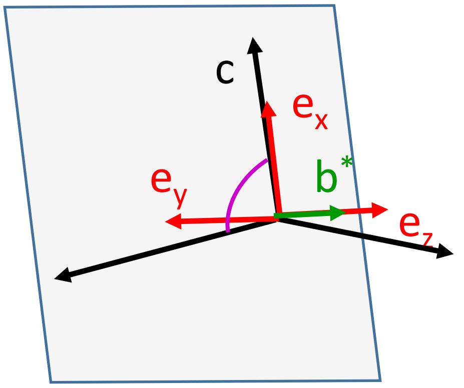
$\cos\alpha^* =$

$$= (\cos\beta \cdot \cos\gamma - \cos\alpha) / (\sin\beta \cdot \sin\gamma)$$

$\cos\gamma^* =$

$$= (\cos\alpha \cdot \cos\beta - \cos\gamma) / (\sin\alpha \cdot \sin\beta)$$





Orthogonalisation matrix :

$$\begin{pmatrix} a \cdot \cos\beta & b \cdot \cos\alpha & c \\ a \cdot \sin\beta & -b \cdot \cos\gamma^* \cdot \sin\alpha & 0 \\ 0 & b \cdot \sin\gamma^* \cdot \sin\alpha & 0 \end{pmatrix}$$

Deorthogonalisation matrix :

$$\begin{pmatrix} 0 & 1/(a \cdot \sin\beta) & 1/(a \cdot \tan\gamma^* \cdot \sin\beta) \\ 0 & 0 & 1/(b \cdot \sin\gamma^* \cdot \sin\alpha) \\ 1/c & -1/(c \cdot \tan\beta) & \sin\gamma \cdot \cos\alpha^* / (c \cdot \sin\gamma^* \cdot \sin\alpha \cdot \sin\beta) \end{pmatrix}$$

$\mathbf{e}_x \parallel (\mathbf{a}+\mathbf{b})$, $\mathbf{e}_y \parallel (\mathbf{c}^* \times (\mathbf{a}+\mathbf{b}))$, $\mathbf{e}_z \parallel \mathbf{c}^*$

Definitions

a, **b**, **c** - *cell axes, cristallographic basis*

a, b, c - cell size

α, β, γ - *cell angles*

$\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ - *orthonormal basis*

$\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ - *conjugate basis*

$\cos\alpha^* =$

$= (\cos\beta\cdot\cos\gamma - \cos\alpha) / (\sin\beta\cdot\sin\gamma)$

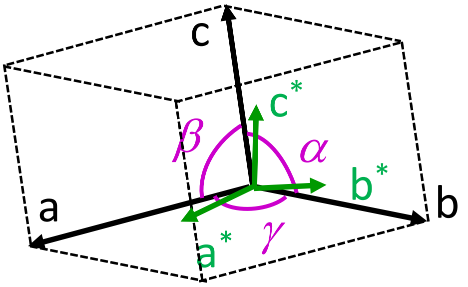
$a' = (a^2+b^2+2ab\cdot\cos\gamma)^{1/2}$

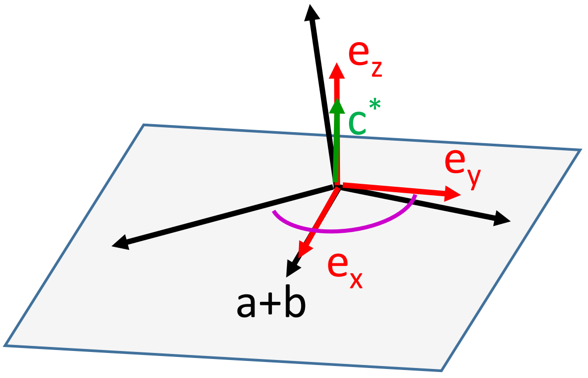
$\cos\beta' = (a\cdot\cos\beta + b\cdot\cos\alpha)/a'$

$\cos\gamma' = (a\cdot\cos\gamma + b)/a'$

$\cos\beta'^* =$

$= (\cos\gamma'\cdot\cos\alpha - \cos\beta') / (\sin\gamma'\cdot\sin\alpha)$





Orthogonalisation matrix :

$$\begin{pmatrix} a' & b\cdot\cos\gamma' & c\cdot\cos\beta' \\ 0 & b\cdot\sin\gamma' & -c\cdot\cos\alpha^*\cdot\sin\beta' \\ 0 & 0 & c\cdot\sin\alpha^*\cdot\sin\beta' \end{pmatrix}$$

Deorthogonalisation matrix :

$$\begin{pmatrix} 1/a' & -1/(a'\cdot\tan\gamma') & \sin\alpha\cdot\cos\beta'^*/(a'\cdot\sin\alpha^*\cdot\sin\beta'\cdot\sin\gamma') \\ 0 & 1/(b\cdot\sin\gamma') & 1/(b\cdot\tan\alpha^*\cdot\sin\gamma') \\ 0 & 0 & 1/(c\cdot\sin\alpha^*\cdot\sin\beta') \end{pmatrix}$$

$\mathbf{e_x} \parallel \mathbf{a^*}$, $\mathbf{e_y} \parallel (\mathbf{c}\times\mathbf{a^*})$, $\mathbf{e_z} \parallel \mathbf{c}$

Definitions

a, **b**, **c** - *cell axes, cristallographic basis*

a, b, c - cell size

α, β, γ - *cell angles*

$\mathbf{e_x}$, $\mathbf{e_y}$, $\mathbf{e_z}$ - *orthonormal basis*

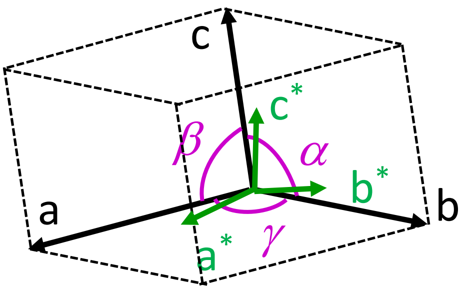
$\mathbf{a^*}$, $\mathbf{b^*}$, $\mathbf{c^*}$ - *conjugate basis*

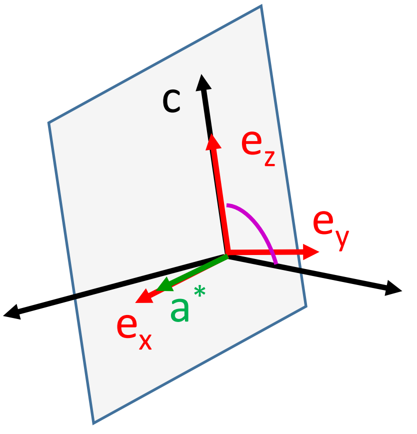
$\cos\beta^* =$

$$= (\cos\gamma\cdot\cos\alpha - \cos\beta) / (\sin\gamma\cdot\sin\alpha)$$

$\cos\gamma^* =$

$$= (\cos\alpha\cdot\cos\beta - \cos\gamma) / (\sin\alpha\cdot\sin\beta)$$





Orthogonalisation matrix :

$$\begin{pmatrix} a\cdot\sin\beta\cdot\sin\gamma^* & 0 & 0 \\ -a\cdot\sin\beta\cdot\cos\gamma^* & b\cdot\sin\alpha & 0 \\ a\cdot\cos\beta & b\cdot\cos\alpha & c \end{pmatrix}$$

Deorthogonalisation matrix :

$$\begin{pmatrix} 1/(a\cdot\sin\beta\cdot\sin\gamma^*) & 0 & 0 \\ 1/(b\cdot\sin\alpha\cdot\tan\gamma^*) & 1/(b\cdot\sin\alpha) & 0 \\ \cos\beta^*\cdot\sin\gamma/(c\cdot\sin\alpha\cdot\sin\beta\cdot\sin\gamma^*) & -1/(c\cdot\tan\alpha) & 1/c \end{pmatrix}$$

$\mathbf{e}_x \parallel \mathbf{a}$, $\mathbf{e}_y \parallel \mathbf{b}^*$, $\mathbf{e}_z \parallel (\mathbf{a}\times\mathbf{b}^*)$

Definitions

a, **b**, **c** - *cell axes, cristallographic basis*

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α, β, γ - *cell angles*

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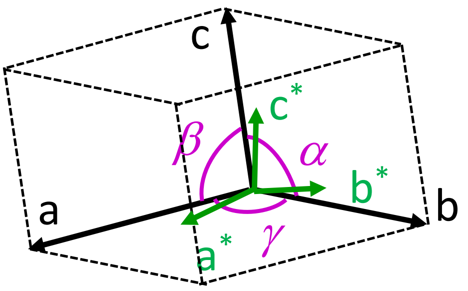
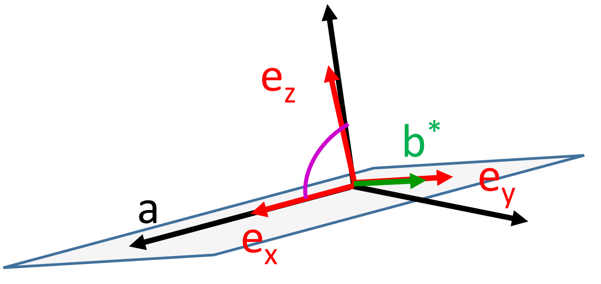
$\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ - *conjugate basis*

$$\cos\alpha^* = (\cos\beta\cdot\cos\gamma-\cos\alpha)/(\sin\beta\cdot\sin\gamma)$$

$$\cos\gamma^* = (\cos\alpha\cdot\cos\beta-\cos\gamma)/(\sin\alpha\cdot\sin\beta)$$





Orthogonalisation matrix :

$$\begin{pmatrix} a & b\cdot\cos\gamma & c\cdot\cos\beta \\ 0 & b\cdot\sin\alpha^*\cdot\sin\gamma & 0 \\ 0 & -b\cdot\cos\alpha^*\cdot\sin\gamma & c\cdot\sin\beta \end{pmatrix}$$

Deorthogonalisation matrix :

$$\begin{pmatrix} 1/a & \sin\alpha\cdot\cos\gamma^*/(a\cdot\sin\alpha^*\cdot\sin\beta\cdot\sin\gamma) & -1/(a\cdot\tan\beta) \\ 0 & 1/(b\cdot\sin\alpha^*\cdot\sin\gamma) & 0 \\ 0 & 1/(c\cdot\tan\alpha^*\cdot\sin\beta) & 1/(c\cdot\sin\beta) \end{pmatrix}$$

$e_x \parallel a^*$, $e_y \parallel b$, $e_z \parallel (a^* \times b)$

Definitions

a, **b**, **c** - *cell axes, cristallographic basis*

a, b, c - cell size

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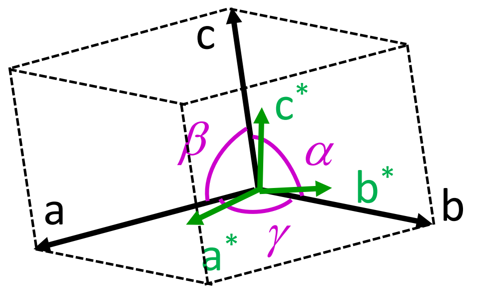
$\mathbf{a^*}$, $\mathbf{b^*}$, $\mathbf{c^*}$ - *conjugate basis*

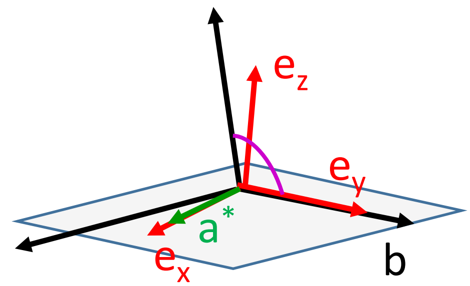
$\cos\beta^* =$

$= (\cos\gamma\cdot\cos\alpha - \cos\beta) / (\sin\gamma\cdot\sin\alpha)$

$\cos\gamma^* =$

$= (\cos\alpha\cdot\cos\beta - \cos\gamma) / (\sin\alpha\cdot\sin\beta)$





Orthogonalisation matrix :

$$\begin{pmatrix} a\cdot\sin\beta^*\cdot\sin\gamma & 0 & 0 \\ a\cdot\cos\gamma & b & c\cdot\cos\alpha \\ -a\cdot\cos\beta^*\cdot\sin\gamma & 0 & c\cdot\sin\alpha \end{pmatrix}$$

Deorthogonalisation matrix :

$$\begin{pmatrix} 1/(a\cdot\sin\beta^*\cdot\sin\gamma) & 0 & 0 \\ \sin\beta\cdot\cos\gamma^* / (b\cdot\sin\alpha\cdot\sin\beta^*\cdot\sin\gamma) & 1/b & -1/(b\cdot\tan\alpha) \\ 1/(c\cdot\sin\alpha\cdot\tan\beta^*) & 0 & 1/(c\cdot\sin\alpha) \end{pmatrix}$$