

# Checking unit cell:

$$\begin{aligned}a &= 3.4\text{\AA}, b = 7.5\text{\AA}, c = 12\text{\AA} \\ \alpha &= 87^\circ, \beta = 102^\circ, \gamma = 124^\circ\end{aligned}\tag{1}$$

## Results

Reciprocal unit cell parameters

$$\begin{aligned}a^* &= 0.36332942\text{\AA}^{-1}, b^* = 0.16133114\text{\AA}^{-1}, c^* = 0.08546101\text{\AA}^{-1} \\ \alpha^* &= 85.47855015^\circ, \beta^* = 77.53862078^\circ, \gamma^* = 55.85213672^\circ\end{aligned}\tag{2}$$

Volume of unit cells:

$$\begin{aligned}V &= 247.36961584064142\text{\AA}^3 \\ V^* &= 0.00404\text{\AA}^{-3}\end{aligned}\tag{3}$$

$$\phi^2 = 0.653506416775028\tag{4}$$

Metric tensors:

$$\mathbf{G}_{\text{direct}} = \begin{bmatrix} 11.56000 & -14.25942 & -8.48280 \\ -14.25942 & 56.25000 & 4.71024 \\ -8.48280 & 4.71024 & 144.00000 \end{bmatrix}\tag{5}$$

$$\mathbf{G}_{\text{direct norm.}} = \begin{bmatrix} 1. & -0.5591929 & -0.20791169 \\ -0.5591929 & 1. & 0.05233596 \\ -0.20791169 & 0.05233596 & 1. \end{bmatrix}\tag{6}$$

$$\mathbf{G}_{\text{recip.}} = \begin{bmatrix} 0.13201 & 0.03290 & 0.00670 \\ 0.03290 & 0.02603 & 0.00109 \\ 0.00670 & 0.00109 & 0.00730 \end{bmatrix}\tag{7}$$

$$\mathbf{G}_{\text{recip.norm.}} = \begin{bmatrix} 1. & 0.56133054 & 0.21578149 \\ 0.56133054 & 1. & 0.07883231 \\ 0.21578149 & 0.07883231 & 1. \end{bmatrix}\tag{8}$$

Matrices:

$$\mathbf{B} = \begin{bmatrix} 0.36332942 & 0.0905601 & 0.0184409 \\ 0 & 0.13351631 & -0.00436731 \\ 0 & 0 & 0.08333333 \end{bmatrix}\tag{9}$$

$$\mathbf{B}^{-1} = \begin{bmatrix} 2.75232 & -1.86682 & -0.70690 \\ 0.00000 & 7.48972 & 0.39252 \\ 0.00000 & 0.00000 & 12.00000 \end{bmatrix}$$

$$\mathbf{B}_{\text{norm}} = \begin{bmatrix} 1.00000 & 0.56133 & 0.21578 \\ 0.00000 & 0.82759 & -0.05110 \\ 0.00000 & 0.00000 & 0.97510 \end{bmatrix} \quad (10)$$

$$\mathbf{B}_{\text{norm}}^{-1} = \begin{bmatrix} 1.00000 & -0.67827 & -0.25684 \\ 0.00000 & 1.20833 & 0.06333 \\ 0.00000 & 0.00000 & 1.02553 \end{bmatrix}$$

$$\mathbf{M} = \begin{bmatrix} 2.75232 & 0.00000 & 0.00000 \\ -1.86682 & 7.48972 & 0.00000 \\ -0.70690 & 0.39252 & 12.00000 \end{bmatrix} \quad (11)$$

$$\mathbf{M}^{-1} = \begin{bmatrix} 0.36333 & 0.00000 & 0.00000 \\ 0.09056 & 0.13352 & 0.00000 \\ 0.01844 & -0.00437 & 0.08333 \end{bmatrix}$$

$$\mathbf{M}_{\text{norm}} = \begin{bmatrix} 0.80951 & 0.00000 & 0.00000 \\ -0.54906 & 0.99863 & 0.00000 \\ -0.20791 & 0.05234 & 1.00000 \end{bmatrix} \quad (12)$$

$$\mathbf{M}_{\text{norm}}^{-1} = \begin{bmatrix} 1.23532 & 0.00000 & 0.00000 \\ 0.67920 & 1.00137 & 0.00000 \\ 0.22129 & -0.05241 & 1.00000 \end{bmatrix}$$

$$\mathbf{M}^{-1} \cdot \mathbf{B}_{\text{norm.}} = \begin{bmatrix} 0.36332942 & 0.203947897 & 0.0783997613 \\ 0.0905600957 & 0.16133114 & 0.0127181067 \\ 0.0184409045 & 0.00673708925 & 0.08546101 \end{bmatrix} \quad (13)$$

$$\mathbf{B}_{\text{norm.}}^{-1} \cdot \mathbf{M} = \begin{bmatrix} 4.20008805 & -5.1808664 & -3.08204968 \\ -2.30048833 & 9.07487662 & 0.75990775 \\ -0.72494843 & 0.40254155 & 12.30638596 \end{bmatrix} \quad (14)$$

## Results for transformations of quadratic form

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Quadratic form in different coordinate systems:

$$\mathbf{Q}_{\text{recip. norm}} = \begin{bmatrix} 3.1 & 0.4 & -0.7 \\ 0.4 & 2.9 & 5.2 \\ -0.7 & 5.2 & 5.7 \end{bmatrix} \quad (15)$$

$$\mathbf{Q}_{\text{XYZ}} = \begin{bmatrix} 3.10000 & -1.61930656 & -1.48873842 \\ -1.61930656 & 5.00464377 & 7.55124895 \\ -1.48873842 & 7.55124895 & 7.24204832 \end{bmatrix} \quad (16)$$

$$\mathbf{Q}_{\text{recip.}} = \begin{bmatrix} 0.40922562 & 0.02344654 & -0.02173535 \\ 0.02344654 & 0.07548044 & 0.07169512 \\ -0.02173535 & 0.07169512 & 0.04163043 \end{bmatrix} \quad (17)$$

$$\mathbf{Q}_{\text{direct}} = \begin{bmatrix} 86.90688 & -152.48631 & -279.76439 \\ -152.48631 & 326.25521 & 712.79278 \\ -279.76439 & 712.79278 & 1042.85496 \end{bmatrix} \quad (18)$$

$$\mathbf{Q}_{\text{direct norm.}} = \begin{bmatrix} 7.51789858 & -5.9798562 & -6.8569725 \\ -5.9798562 & 5.80008894 & 7.91992089 \\ -6.8569725 & 7.91992089 & 7.24205 \end{bmatrix} \quad (19)$$

For reflections:

$$\text{refln\_hkl} = \begin{bmatrix} 0 & 0 & 2 \\ 0 & 2 & 0 \\ 2 & 0 & 0 \\ 2 & 2 & 2 \\ 1 & 2 & 3 \end{bmatrix} \quad (20)$$

$$\text{q\_ccs} = \begin{bmatrix} 0.21578149 & -0.05110301 & 0.9751035 \\ 0.56133054 & 0.8275917 & 0. \\ 1. & 0. & 0. \\ 0.95091959 & 0.26000932 & 0.1677709 \\ 0.85971072 & 0.363983 & 0.35834878 \end{bmatrix} \quad (21)$$

$$d^{-1} = \begin{bmatrix} 0.17092203 \\ 0.32266228 \\ 0.72665883 \\ 0.99250719 \\ 0.68715675 \end{bmatrix} \quad (22)$$

$$\frac{\sin \theta}{\lambda} = \begin{bmatrix} 0.08546101 \\ 0.16133114 \\ 0.36332942 \\ 0.49625359 \\ 0.34357837 \end{bmatrix} \quad (23)$$