Formation, Structure, and Frequency-Doubling Effect of a Modification of Strontium Cyanurate (α-SCY)

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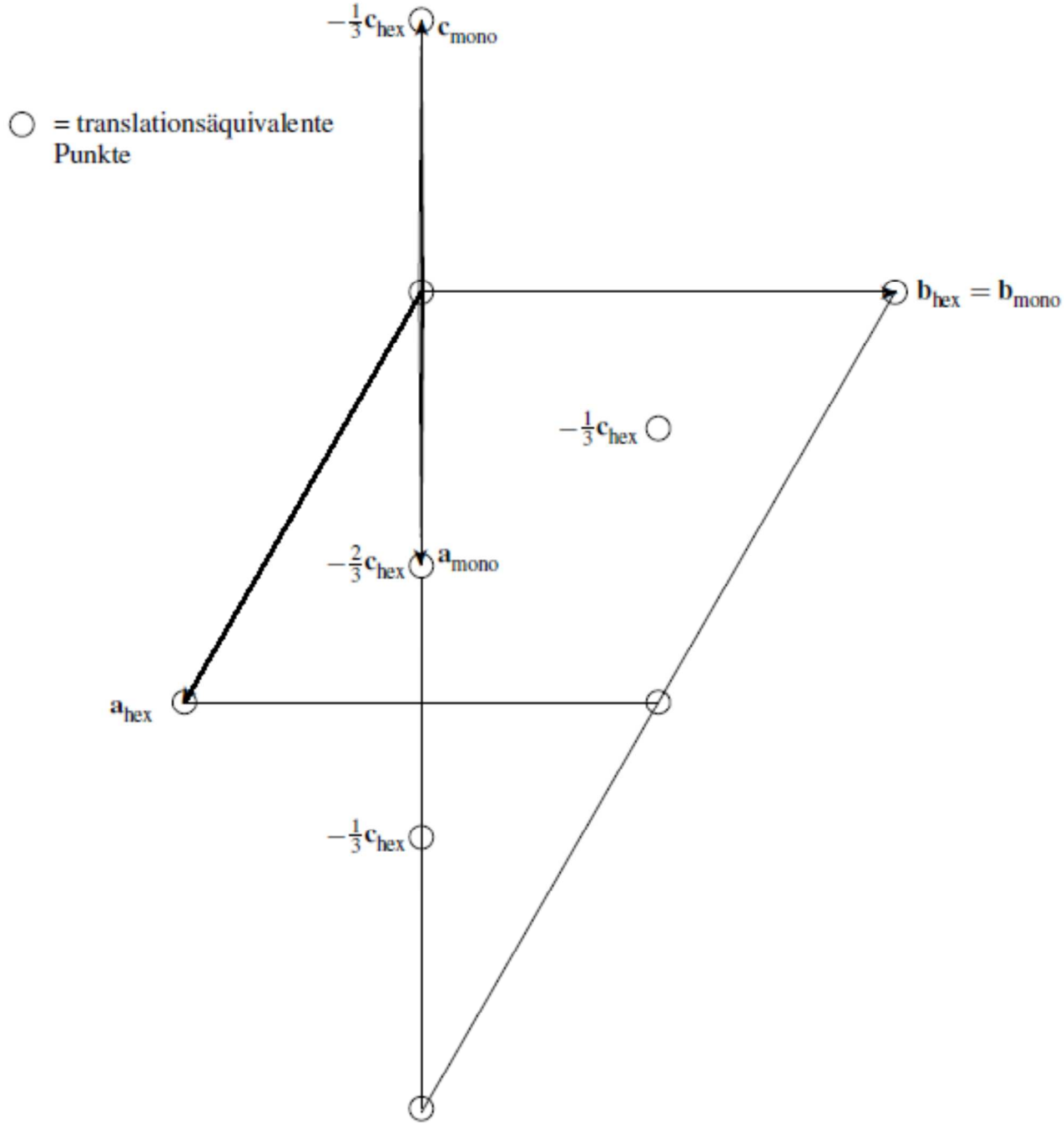

Figure S1. Graphic for unit cell transformation.

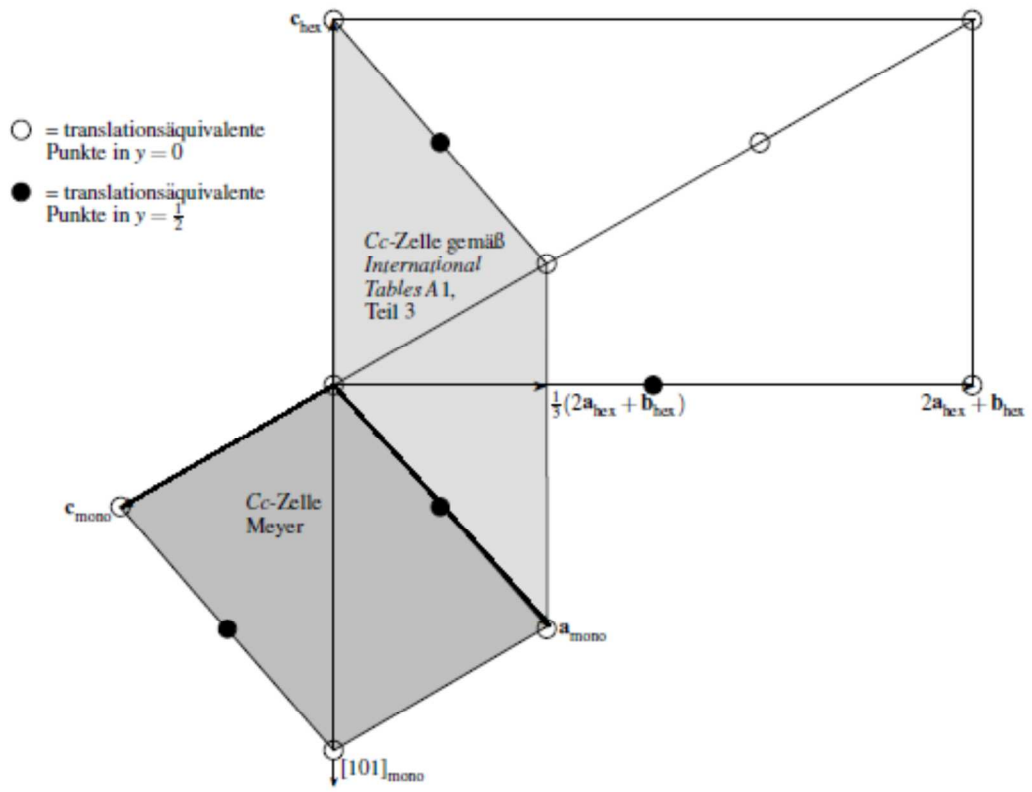

Figure S2. Geometric relationship between rhombohedral and monoclinic unit cell.

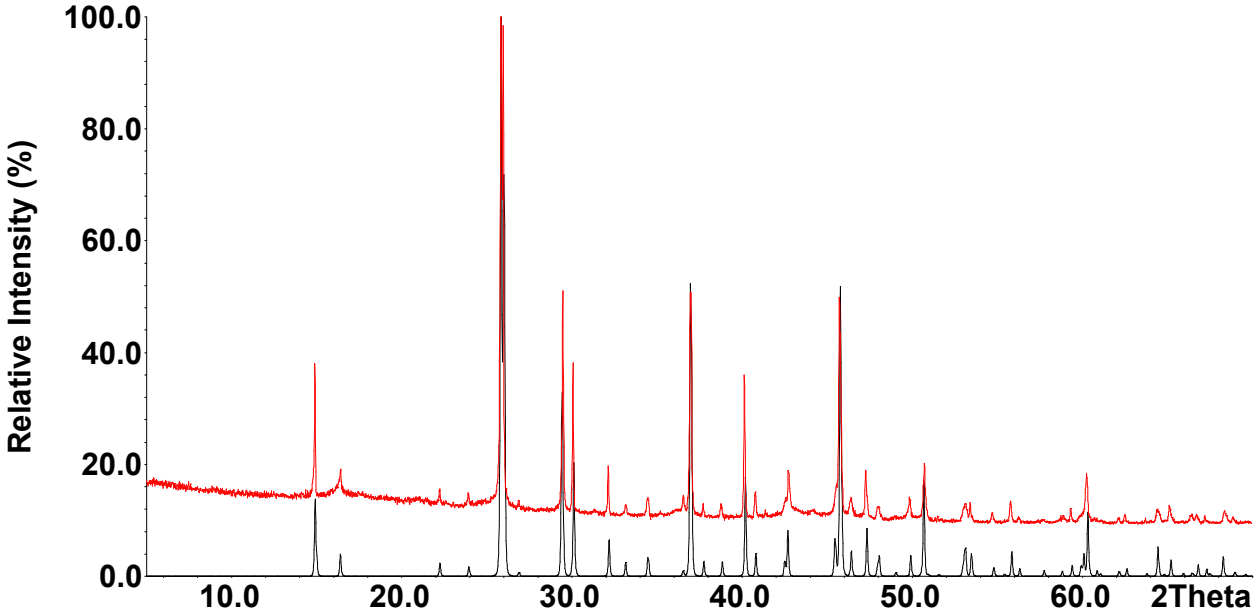

Figure S3. Powder diffraction pattern of phase pure β-SCY. Theoretical pattern simulated from crystallographic data (black) and recorded pattern (red).

$$(\mathbf{a},\mathbf{b},\mathbf{c})_{Cc} = (\mathbf{a},\mathbf{b},\mathbf{c})_{R3c} \begin{pmatrix} \frac{2}{3} & 0 & -\frac{2}{3} \\ \frac{1}{3} & -1 & -\frac{1}{3} \\ -\frac{2}{3} & 0 & -\frac{1}{3} \end{pmatrix}$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}_{Cc} = \begin{pmatrix} \frac{1}{2} & 0 & -1 \\ \frac{1}{2} & -1 & 0 \\ -1 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_{R3c} - \begin{pmatrix} 0 \\ \frac{1}{4} \\ 0 \end{pmatrix}$$

Equation S1 and S2 for the transformation of lattice parameters (top) and atomic coordinates from *R3c* to *Cc* (bottom).