

When to convert Cc to Ia or $C2/c$ to $I2/a$ (or inverse see below)

Convention $a < c$ and β near 90° .

If the C cell has $a > c$ and $\beta > 120^\circ$ then convert to the I cell

Convert Monoclinic $C \rightarrow I$

Direct cell axes and HKL transformation matrix :

$$\begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

Coordinate transformation matrix :

$$\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

If the I cell has $a > c$ and $\beta > 120^\circ$ then convert to the C cell

Convert Monoclinic $I \rightarrow C$

Direct cell axes and HKL transformation matrix :

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

Coordinate transformation matrix :

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

Mighell A. D. (2002). Conventional Cells-The Last Step Toward General Acceptance of Standard Conventional Cells for the Reporting of Crystallographic Data. *Journal of research of the National Institute of Standards and Technology*, 107(4), 373–377. <https://doi.org/10.6028/jres.107.030>