$$(1)\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix};\quad (2)\begin{pmatrix}\bar{1}&0&0&\bar{\frac{1}{2}}\\0&\bar{1}&0&0\\0&0&1&\frac{1}{2}\\0&0&0&1\end{pmatrix};\quad (3)\begin{pmatrix}0&\bar{1}&0&\frac{1}{4}\\1&0&0&\frac{1}{4}\\0&0&1&\frac{1}{4}\\0&0&0&1\end{pmatrix};$$

$$(4)\begin{pmatrix}0&1&0&\frac{1}{4}\\\bar{1}&0&0&\bar{\frac{1}{4}}\\0&0&1&\frac{3}{4}\\0&0&0&1\end{pmatrix};\quad (5)\begin{pmatrix}0&1&0&\frac{1}{4}\\1&0&0&\frac{1}{4}\\0&0&\bar{1}&\frac{1}{4}\\0&0&0&1\end{pmatrix};\quad (6)\begin{pmatrix}0&\bar{1}&0&\frac{1}{4}\\\bar{1}&0&0&\bar{\frac{1}{4}}\\0&0&\bar{1}&\frac{3}{4}\\0&0&0&1\end{pmatrix};$$

$$(7)\begin{pmatrix}1&0&0&0\\0&\bar{1}&0&0\\0&0&\bar{1}&0\\0&0&0&1\end{pmatrix};\quad (8)\begin{pmatrix}\bar{1}&0&0&\bar{\frac{1}{2}}\\0&1&0&0\\0&0&\bar{1}&\frac{1}{2}\\0&0&0&1\end{pmatrix}.$$

Another set of eight matrices is obtained by adding the *C*-centring translation $\frac{1}{2}, \frac{1}{2}, 0$ to the ***w***'s.

From these matrices, one obtains the coordinates of the general position in the *C* cell, for instance from matrix (2)

$$\begin{pmatrix}\tilde{x}\\\tilde{y}\\\tilde{z}\\1\end{pmatrix}=\begin{pmatrix}\bar{1}&0&0&\bar{\frac{1}{2}}\\0&\bar{1}&0&0\\0&0&1&\frac{1}{2}\\0&0&0&1\end{pmatrix}\begin{pmatrix}x\\y\\z\\1\end{pmatrix}=\begin{pmatrix}-x-\frac{1}{2}\\-y\\z+\frac{1}{2}\\1\end{pmatrix}.$$

The eight points obtained by the eight matrices $\mathbb{W}'$ are

(1)	$x, y, z;$	(2)	$-\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z;$
(3)	$\frac{1}{4}-y, \frac{1}{4}+x, \frac{1}{4}+z;$	(4)	$\frac{1}{4}+y, -\frac{1}{4}-x, \frac{3}{4}+z;$
(5)	$\frac{1}{4}+y, \frac{1}{4}+x, \frac{1}{4}-z;$	(6)	$\frac{1}{4}-y, -\frac{1}{4}-x, \frac{3}{4}-z;$
(7)	$x, \bar{y}, \bar{z};$	(8)	$-\frac{1}{2}-x, y, \frac{1}{2}-z.$

The other set of eight points is obtained by adding $\frac{1}{2}, \frac{1}{2}, 0$.

In space group $P4_12_12$, the silicon atoms are in special position $4(a)$ ..2 with the coordinates $x, x, 0$. Transformed into the *C* cell, the position becomes

$$\begin{array}{llll}(0,0,0)+ & (\frac{1}{2},\frac{1}{2},0)+ & & \\ x,0,0; & \frac{1}{2}-x,0,\frac{1}{2}; & \frac{1}{4},\frac{1}{4}+x,\frac{1}{4}; & \frac{1}{4},\frac{3}{4}-x,\frac{3}{4}.\end{array}$$

The parameter $x = 0.300$ of the *P* cell has changed to $x = 0.050$ in the *C* cell. For $x = 0$, the special position of the *C* cell assumes the same coordinate triplets as Wyckoff position $8(a)$ $\bar{4}3m$ in space group $Fd\bar{3}m$ (227), *i.e.* this change of the *x* parameter reflects the displacement of the silicon atoms in the cubic to tetragonal phase transition.

References

5.2

Altmann, S. L. & Herzig, P. (1994). *Point-Group Theory Tables*. Oxford Science Publications.

International Tables for Crystallography (2004). Vol. C, edited by E. Prince, Table 8.3.1.1. Dordrecht: Kluwer Academic Publishers.

Megaw, H. D. (1973). *Crystal structures: a working approach*, pp. 259–262. Philadelphia: Saunders.

Nieuwenkamp, W. (1935). *Die Kristallstruktur des Tief-Cristobalits SiO_2. Z. Kristallogr.* **92**, 82–88.

Wyckoff, R. W. G. (1925). *Die Kristallstruktur von β-Cristobalit SiO_2 (bei hohen Temperaturen stabile Form). Z. Kristallogr.* **62**, 189–200.