International Tables for Crystallography (2016). Vol. A, Table 1.5.1.1, pp. 77–80.

Table 1.5.1.1
Selected 3×3 transformation matrices $\boldsymbol{P}$ and $\boldsymbol{Q} = \boldsymbol{P}^{-1}$

For inverse transformations (against the arrow) replace $\boldsymbol{P}$ by $\boldsymbol{Q}$ and *vice versa.*

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ C \to A \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ A \to I \end{cases}$ Unique axis **b** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to C \end{cases}$ (Fig. 1.5.1.2*a*)	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ B \to I \end{cases}$ Unique axis **c** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to A \end{cases}$ (Fig. 1.5.1.2*b*)	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ B \to C \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ C \to I \end{cases}$ Unique axis **a** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to B \end{cases}$ (Fig. 1.5.1.2*c*)	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **b** → unique axis **c** Cell choice 1: $\begin{cases} P \to P \\ C \to A \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **b** → unique axis **a** Cell choice 1: $\begin{cases} P \to P \\ C \to B \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ A \to C \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **c** → unique axis **a** Cell choice 1: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ B \to C \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
$I \to P$ (Fig. 1.5.1.3)	$\begin{pmatrix} \bar{\frac{1}{2}} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \bar{\frac{1}{2}} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \bar{\frac{1}{2}} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	Orthorhombic Tetragonal Cubic
$F \to P$ (Fig. 1.5.1.4)	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	Orthorhombic Tetragonal Cubic

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q}=\boldsymbol{P}^{-1}$	Crystal system
$(\mathbf{b},\mathbf{a},\bar{\mathbf{c}})\rightarrow(\mathbf{a},\mathbf{b},\mathbf{c})$	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar{1}\end{pmatrix}$	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&\bar{1}\end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{c},\mathbf{a},\mathbf{b})\rightarrow(\mathbf{a},\mathbf{b},\mathbf{c})$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	Unconventional orthorhombic setting
$(\bar{\mathbf{c}},\mathbf{b},\mathbf{a})\rightarrow(\mathbf{a},\mathbf{b},\mathbf{c})$	$\begin{pmatrix}0&0&\bar{1}\\0&1&0\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&1&0\\\bar{1}&0&0\end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{b},\mathbf{c},\mathbf{a})\rightarrow(\mathbf{a},\mathbf{b},\mathbf{c})$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{a},\bar{\mathbf{c}},\mathbf{b})\rightarrow(\mathbf{a},\mathbf{b},\mathbf{c})$	$\begin{pmatrix}1&0&0\\0&0&\bar{1}\\0&1&0\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&1\\0&\bar{1}&0\end{pmatrix}$	Unconventional orthorhombic setting
$\left.\begin{matrix}P\rightarrow C_1\\ I\rightarrow F_1\end{matrix}\right\}$ (Fig. 1.5.1.5), **c** axis invariant	$\begin{pmatrix}1&1&0\\\bar{1}&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\bar{\frac{1}{2}}&0\\\frac{1}{2}&\frac{1}{2}&0\\0&0&1\end{pmatrix}$	Tetragonal (*cf.* Section 1.5.4.3)
$\left.\begin{matrix}P\rightarrow C_2\\ I\rightarrow F_2\end{matrix}\right\}$ (Fig. 1.5.1.5), **c** axis invariant	$\begin{pmatrix}1&\bar{1}&0\\1&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0\\\bar{\frac{1}{2}}&\frac{1}{2}&0\\0&0&1\end{pmatrix}$	Tetragonal (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → triple hexagonal cell R_1, obverse setting (Fig. 1.5.1.6*a*,*c*)	$\begin{pmatrix}1&0&1\\\bar{1}&1&1\\0&\bar{1}&1\end{pmatrix}$	$\begin{pmatrix}\frac{2}{3}&\bar{\frac{1}{3}}&\bar{\frac{1}{3}}\\\frac{1}{3}&\frac{1}{3}&\bar{\frac{2}{3}}\\\frac{1}{3}&\frac{1}{3}&\frac{1}{3}\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → triple hexagonal cell R_2, obverse setting (Fig. 1.5.1.6*c*)	$\begin{pmatrix}0&\bar{1}&1\\1&0&1\\\bar{1}&1&1\end{pmatrix}$	$\begin{pmatrix}\bar{\frac{1}{3}}&\frac{2}{3}&\bar{\frac{1}{3}}\\\bar{\frac{2}{3}}&\frac{1}{3}&\frac{1}{3}\\\frac{1}{3}&\frac{1}{3}&\frac{1}{3}\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → triple hexagonal cell R_3, obverse setting (Fig. 1.5.1.6*c*)	$\begin{pmatrix}\bar{1}&1&1\\0&\bar{1}&1\\1&0&1\end{pmatrix}$	$\begin{pmatrix}\bar{\frac{1}{3}}&\bar{\frac{1}{3}}&\frac{2}{3}\\\frac{1}{3}&\bar{\frac{2}{3}}&\frac{1}{3}\\\frac{1}{3}&\frac{1}{3}&\frac{1}{3}\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → triple hexagonal cell R_1, reverse setting (Fig. 1.5.1.6*d*)	$\begin{pmatrix}\bar{1}&0&1\\1&\bar{1}&1\\0&1&1\end{pmatrix}$	$\begin{pmatrix}\bar{\frac{2}{3}}&\frac{1}{3}&\frac{1}{3}\\\bar{\frac{1}{3}}&\bar{\frac{1}{3}}&\frac{2}{3}\\\frac{1}{3}&\frac{1}{3}&\frac{1}{3}\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → triple hexagonal cell R_2, reverse setting (Fig. 1.5.1.6*b*,*d*)	$\begin{pmatrix}0&1&1\\\bar{1}&0&1\\1&\bar{1}&1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{3}&\bar{\frac{2}{3}}&\frac{1}{3}\\\frac{2}{3}&\bar{\frac{1}{3}}&\bar{\frac{1}{3}}\\\frac{1}{3}&\frac{1}{3}&\frac{1}{3}\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → triple hexagonal cell R_3, reverse setting (Fig. 1.5.1.6*d*)	$\begin{pmatrix}1&\bar{1}&1\\0&1&1\\\bar{1}&0&1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{3}&\frac{1}{3}&\bar{\frac{2}{3}}\\\bar{\frac{1}{3}}&\frac{2}{3}&\bar{\frac{1}{3}}\\\frac{1}{3}&\frac{1}{3}&\frac{1}{3}\end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Hexagonal cell P → orthohexagonal centred cell C_1 (Fig. 1.5.1.7)	$\begin{pmatrix}1&1&0\\0&2&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}1&\bar{\frac{1}{2}}&0\\0&\frac{1}{2}&0\\0&0&1\end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell P → orthohexagonal centred cell C_2 (Fig. 1.5.1.7)	$\begin{pmatrix}1&\bar{1}&0\\1&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{1}{2}&0\\\bar{\frac{1}{2}}&\frac{1}{2}&0\\0&0&1\end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Hexagonal cell $P \rightarrow$ orthohexagonal centred cell C_3 (Fig. 1.5.1.7)	$\begin{pmatrix} 0 & \bar{2} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \overline{\tfrac{1}{2}} & 1 & 0 \\ \overline{\tfrac{1}{2}} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_1 (Fig. 1.5.1.8)	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \tfrac{2}{3} & \overline{\tfrac{1}{3}} & 0 \\ \tfrac{1}{3} & \tfrac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_2 (Fig. 1.5.1.8)	$\begin{pmatrix} 2 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \tfrac{1}{3} & \tfrac{1}{3} & 0 \\ \overline{\tfrac{1}{3}} & \tfrac{2}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_3 (Fig. 1.5.1.8)	$\begin{pmatrix} 1 & \bar{2} & 0 \\ 2 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \overline{\tfrac{1}{3}} & \tfrac{2}{3} & 0 \\ \overline{\tfrac{2}{3}} & \tfrac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple rhombohedral cell D_1	$\begin{pmatrix} 1 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \tfrac{2}{3} & \overline{\tfrac{1}{3}} & \tfrac{1}{3} \\ \overline{\tfrac{1}{3}} & \tfrac{2}{3} & \tfrac{1}{3} \\ \overline{\tfrac{1}{3}} & \overline{\tfrac{1}{3}} & \tfrac{1}{3} \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple rhombohedral cell D_2	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & \bar{1} & 1 \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \overline{\tfrac{2}{3}} & \tfrac{1}{3} & \tfrac{1}{3} \\ \tfrac{1}{3} & \overline{\tfrac{2}{3}} & \tfrac{1}{3} \\ \tfrac{1}{3} & \tfrac{1}{3} & \tfrac{1}{3} \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \tfrac{2}{3} & 0 & 0 \\ \tfrac{1}{3} & 1 & 0 \\ \overline{\tfrac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \tfrac{3}{2} & 0 & 0 \\ \overline{\tfrac{1}{2}} & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \overline{\tfrac{1}{3}} & \bar{1} & 0 \\ \tfrac{1}{3} & \bar{1} & 0 \\ \overline{\tfrac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \overline{\tfrac{3}{2}} & \tfrac{3}{2} & 0 \\ \overline{\tfrac{1}{2}} & \overline{\tfrac{1}{2}} & 0 \\ \bar{1} & 1 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \overline{\tfrac{1}{3}} & 1 & 0 \\ \overline{\tfrac{2}{3}} & 0 & 0 \\ \overline{\tfrac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \overline{\tfrac{3}{2}} & 0 \\ 1 & \overline{\tfrac{1}{2}} & 0 \\ 0 & \bar{1} & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \tfrac{2}{3} & 0 \\ 0 & \tfrac{1}{3} & 1 \\ 1 & \overline{\tfrac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 1 \\ \tfrac{3}{2} & 0 & 0 \\ \overline{\tfrac{1}{2}} & 1 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \overline{\tfrac{1}{3}} & \bar{1} \\ 0 & \tfrac{1}{3} & \bar{1} \\ 1 & \overline{\tfrac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ \overline{\tfrac{3}{2}} & \tfrac{3}{2} & 0 \\ \overline{\tfrac{1}{2}} & \overline{\tfrac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \overline{\tfrac{1}{3}} & 1 \\ 0 & \overline{\tfrac{2}{3}} & 0 \\ 1 & \overline{\tfrac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 1 \\ 0 & \overline{\tfrac{3}{2}} & 0 \\ 1 & \overline{\tfrac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \overline{\tfrac{1}{2}} & \overline{\tfrac{1}{2}} \\ 0 & \tfrac{1}{2} & \overline{\tfrac{1}{2}} \\ 1 & 0 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} \bar{1} & \bar{1} & 1 \\ 0 & 0 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \overline{\tfrac{1}{2}} & 1 & \overline{\tfrac{1}{2}} \\ \overline{\tfrac{1}{2}} & 0 & \tfrac{1}{2} \\ 0 & 1 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Primitive rhombohedral cell → *C*-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 1 \\ \frac{1}{2} & \bar{\frac{1}{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig.1.5.1.10*b*)	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{\frac{1}{2}} & \bar{\frac{1}{2}} \\ 0 & \frac{1}{2} & \bar{\frac{1}{2}} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 1.5.1.10*b*)	$\begin{pmatrix} 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \\ 1 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{\frac{1}{2}} & 1 & \bar{\frac{1}{2}} \\ \bar{\frac{1}{2}} & 0 & \frac{1}{2} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 1.5.1.10*b*)	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 1 \\ \frac{1}{2} & \bar{\frac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)

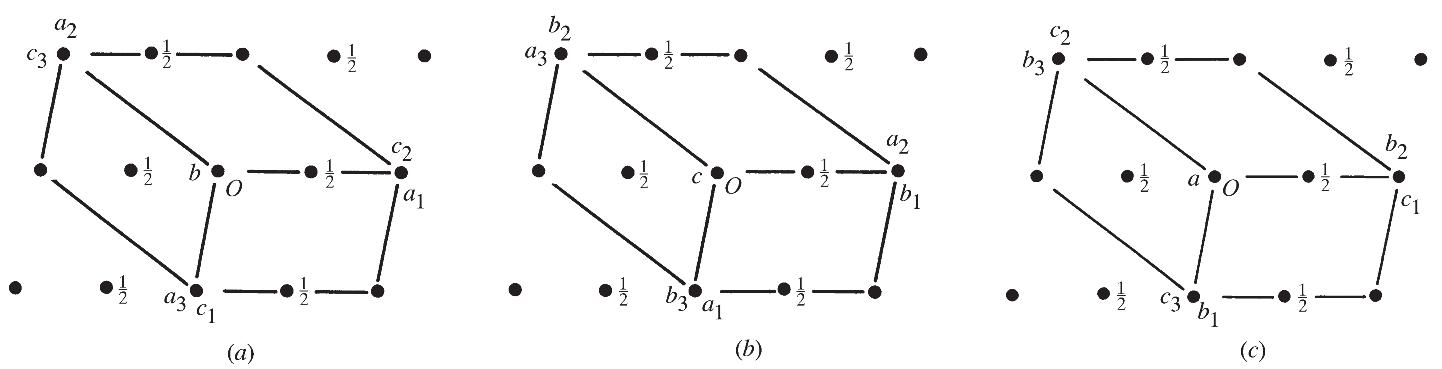

Figure 1.5.1.2
Monoclinic centred lattice, projected along the unique axis. The origin for all the cells is the same. The fractions $\frac{1}{2}$ indicate the height of the lattice points along the axis of projection.

(*a*) Unique axis *b*:
Cell choice 1: *C*-centred cell a_1, b, c_1.
Cell choice 2: *A*-centred cell a_2, b, c_2.
Cell choice 3: *I*-centred cell a_3, b, c_3.

(*b*) Unique axis *c*:
Cell choice 1: *A*-centred cell a_1, b_1, c.
Cell choice 2: *B*-centred cell a_2, b_2, c.
Cell choice 3: *I*-centred cell a_3, b_3, c.

(*c*) Unique axis *a*:
Cell choice 1: *B*-centred cell a, b_1, c_1.
Cell choice 2: *C*-centred cell a, b_2, c_2.
Cell choice 3: *I*-centred cell a, b_3, c_3.

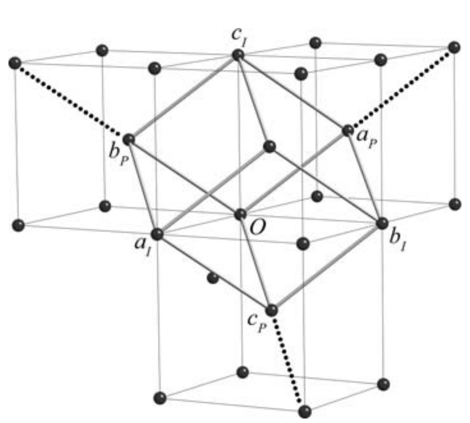

Figure 1.5.1.3
Body-centred cell *I* with a_I, b_I, c_I and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *I* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{3}$ and $\alpha = 109.47°$ (rhombohedral axes) or a triple hexagonal cell with $a_{\rm hex} = a_c\sqrt{2}$ and $c_{\rm hex} = a_c \frac{1}{2}\sqrt{3}$ (hexagonal axes).

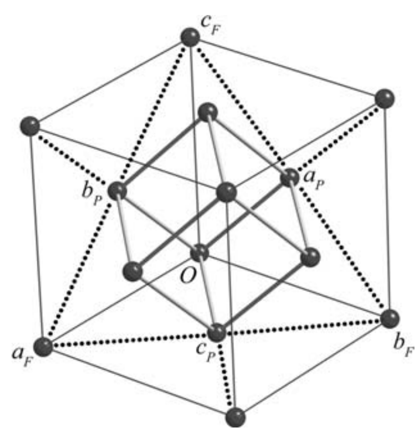

Figure 1.5.1.4
Face-centred cell *F* with a_F, b_F, c_F and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *F* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{2}$ and $\alpha = 60°$ (rhombohedral axes) or a triple hexagonal cell with $a_{\rm hex} = a_c \frac{1}{2}\sqrt{2}$ and $c_{\rm hex} = a_c\sqrt{3}$ (hexagonal axes).