*International Tables for Crystallography* (2010). Vol. B, Figure 4.6.3.33, p. 617.



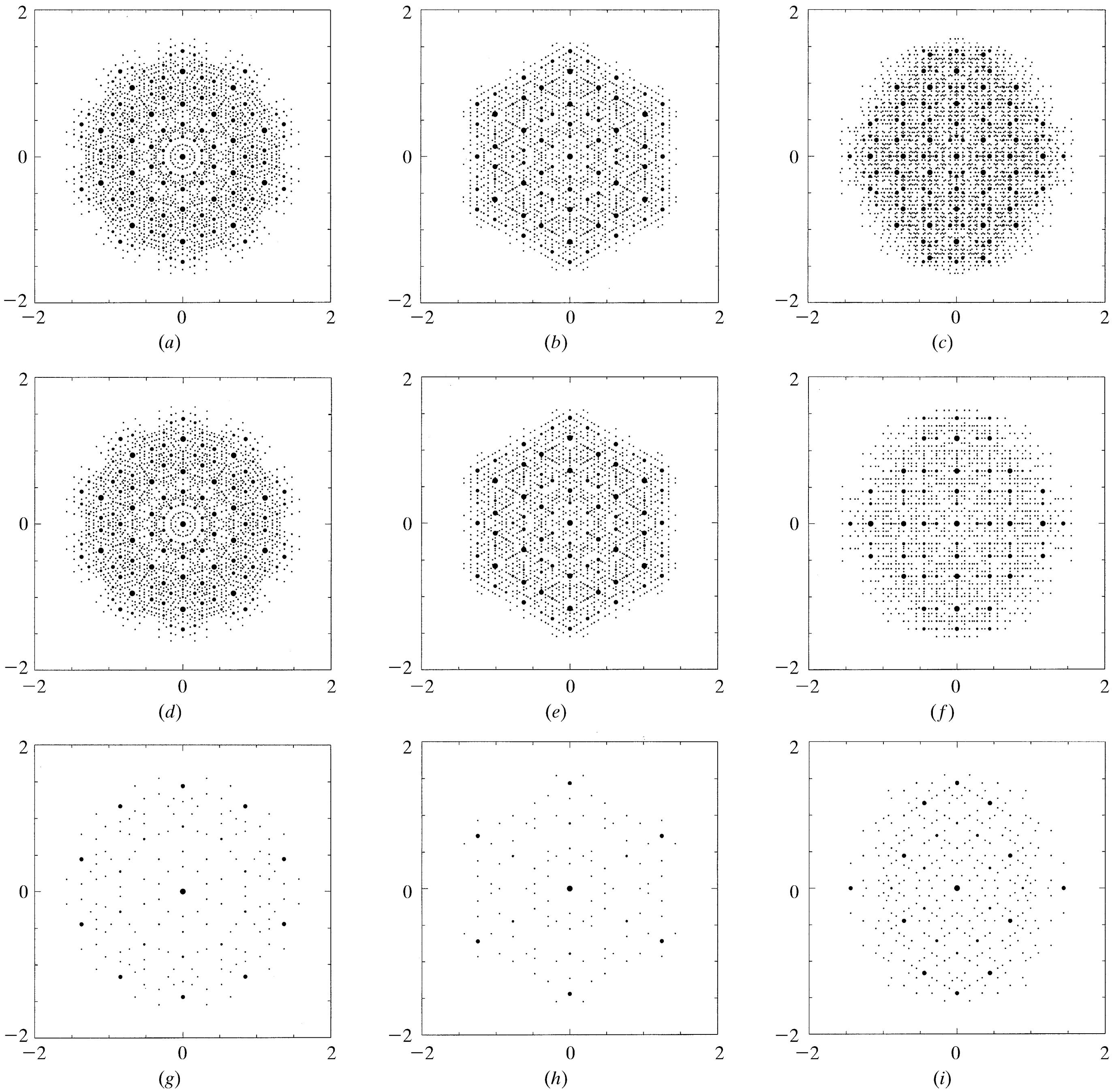


Fig. 4.6.3.33. Physical-space diffraction patterns of the 3D Penrose tiling decorated with point atoms (edge lengths of the Penrose unit rhombohedra $a_r = 5.0$ Å). Sections with five-, three- and twofold symmetry are shown for the primitive 6D analogue of Bravais type $P$ in ($a$, $b$, $c$), the body-centred 6D analogue to Bravais type $I$ in ($d$, $e$, $f$) and the face-centred 6D analogue to Bravais type $F$ in ($g$, $h$, $i$). All reflections are shown within $10^{-4}|F(\mathbf{0})|^2 < |F(\mathbf{H})|^2 < |F(\mathbf{0})|^2$ and $-6 \leq h_i \leq 6, i = 1, \ldots, 6$.

$$\begin{pmatrix} \mathbf{b}_1^* \\ \mathbf{b}_2^* \\ \mathbf{b}_3^* \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & \bar{1} & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}_D \begin{pmatrix} \mathbf{a}_1^* \\ \mathbf{a}_2^* \\ \mathbf{a}_3^* \\ \mathbf{a}_4^* \\ \mathbf{a}_5^* \\ \mathbf{a}_6^* \end{pmatrix}$$

$$= \frac{a^*}{(1+\tau^2)^{1/2}} \begin{pmatrix} \mathbf{e}_1^C \\ \mathbf{e}_2^C \\ \mathbf{e}_3^C \end{pmatrix}.$$

The Cartesian $C$ basis is related to the $V$ basis by a $\theta/2$ rotation around $[100]_C$, yielding $[001]_V$, followed by a $\pi/10$ rotation around $[001]_C$:

$$\begin{pmatrix} \mathbf{e}_1^C \\ \mathbf{e}_2^C \\ \mathbf{e}_3^C \end{pmatrix} = \begin{pmatrix} \cos(\pi/10) & \sin(\pi/10) & 0 \\ -\cos(\theta/2)\sin(\pi/10) & \cos(\theta/2)\cos(\pi/10) & \sin(\theta/2) \\ \sin(\theta/2)\sin(\pi/10) & -\sin(\theta/2)\cos(\pi/10) & \cos(\theta/2) \end{pmatrix}_V \begin{pmatrix} \mathbf{e}_1^V \\ \mathbf{e}_2^V \\ \mathbf{e}_3^V \end{pmatrix}.$$

Thus, indexing the diffraction pattern of an icosahedral phase with integer indices, one obtains for setting 1 $\mathbf{H} = \sum_{i=1}^{6} h_i \mathbf{a}_i^*$, $h_i \in \mathbb{Z}$. These indices $(h_1\ h_2\ h_3\ h_4\ h_5\ h_6)$ transform into the second setting to $(h/h'\ k/k'\ l/l')$ with the fractional cubic indices $h_1^c = h + h'\tau$, $h_2^c = k + k'\tau$, $h_3^c = l + l'\tau$. The transformation matrix is



references