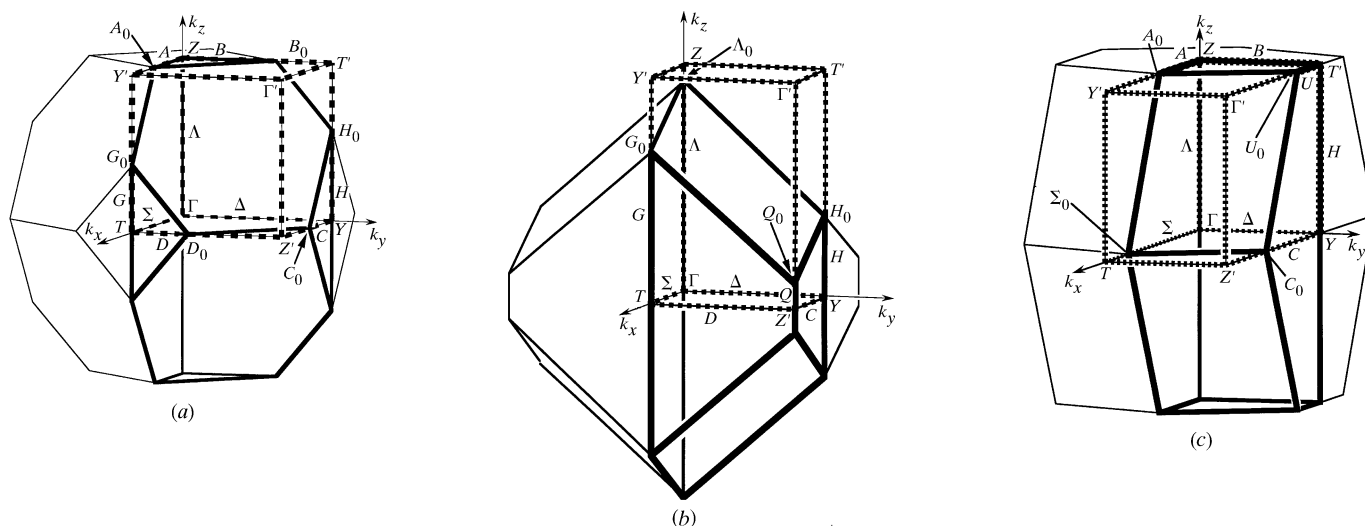


1.5. CLASSIFICATION OF SPACE-GROUP REPRESENTATIONS


 Fig. 1.5.5.4. Symmorphic space group $Imm2$ (isomorphic to the reciprocal-space group \mathcal{G}^* of $mm2F$).

(a) Brillouin zone (thin lines), representation domain (thick lines) and asymmetric unit (dashed lines, partly protruding) imbedded in the Brillouin zone, which is an orthorhombic cuboctahedron. The diagram is drawn for $a^{*2} = 9$, $b^{*2} = 8$, $c^{*2} = 7$, i.e. $a^{*2} + b^{*2} > c^{*2}$. The endpoint of line A is A_0 etc., the free coordinate of A_0 is a_0 etc. Asymmetric unit $\Gamma TZ'YZY'\Gamma T'$ of $Imm2$, IT A, p. 246. The part $\Gamma TD_0C_0YG_0H_0ZA_0B_0$ is common to both bodies; the part $A_0Y'\Gamma T'B_0G_0H_0D_0Z'C_0$ is equivalent to the part of the representation domain with negative z values through a twofold screw rotation 2_1 around the axis $\frac{1}{4}, \frac{1}{4}, z$. Coordinates of the points: $\Gamma = 0, 0, 0 \sim \Gamma' = \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; $Y = 0, \frac{1}{2}, 0 \sim Y' = \frac{1}{2}, 0, \frac{1}{2}$; $Z = 0, 0, \frac{1}{2} \sim Z' = \frac{1}{2}, \frac{1}{2}, 0$; $T = \frac{1}{2}, 0, 0 \sim T' = 0, \frac{1}{2}, \frac{1}{2}$; $C_0 = c_0, \frac{1}{2}, 0 \sim A_0 = a_0, 0, \frac{1}{2}$; $D_0 = \frac{1}{2}, d_0, 0 \sim B_0 = 0, b_0, \frac{1}{2}$; $G_0 = \frac{1}{2}, 0, g_0 \sim H_0 = 0, \frac{1}{2}, h_0$. The coordinates of the points are $c_0 = 1/4[1 - (b^{*2} - c^{*2})/a^{*2}]$; $a_0 = 1/2 - c_0$; $d_0 = 1/4[1 - (a^{*2} - c^{*2})/b^{*2}]$; $b_0 = 1/2 - d_0$; $g_0 = 1/4[1 - (a^{*2} - b^{*2})/c^{*2}]$; $h_0 = 1/2 - g_0$. The sign \sim means symmetrically equivalent. There are no special points. The points Γ, T, Y, Z, G_0 and H_0 belong to special lines; A_0, B_0, C_0 and D_0 belong to special planes. The points with negative z coordinates are equivalent to those already listed. Lines: $\Lambda = \Gamma Z = 0, 0, z$; $G = TG_0 = \frac{1}{2}, 0, z$; $H = YH_0 = 0, \frac{1}{2}, z$. The lines $\Sigma = \Gamma T = x, 0, 0$; $C = YC_0 = x, \frac{1}{2}, 0$; $A = ZA_0 = x, 0, \frac{1}{2}$; $\Delta = \Gamma Y = 0, y, 0$; $B = ZB_0 = 0, y, \frac{1}{2}$; $D = TD_0 = \frac{1}{2}, y, 0$; A_0G_0, G_0D_0, C_0H_0 and H_0B_0 have no special symmetry but belong to special planes, the lines D_0C_0 and B_0A_0 belong to the general position GP . The lines $\Gamma Z, TG_0, YH_0, D_0G_0, C_0H_0, G_0A_0, H_0B_0, ZA_0, ZB_0$ and A_0B_0 of the representation domain to the points Z, G_0, H_0, A_0 and B_0 with negative z coordinates are equivalent to lines of the asymmetric unit not belonging to the representation domain. Planes: $E = \Gamma YH_0B_0Z = 0, y, z$; $F = TD_0G_0 = \frac{1}{2}, y, z$; $J = \Gamma ZA_0G_0T = x, 0, z$; $K = YH_0C_0 = x, \frac{1}{2}, z$. The planes $x, y, 0$; $x, y, \frac{1}{2}$; and $D_0C_0H_0B_0A_0G_0$ belong to the general position GP , as do the negative counterparts of the latter two. The planes $\Gamma Z\bar{A}_0\bar{G}_0T, \Gamma Z\bar{B}_0\bar{H}_0Y, Y\bar{H}_0\bar{C}_0$ and $T\bar{D}_0\bar{G}_0$ of the representation domain to the points Z, A_0, B_0, G_0 and H_0 with negative z coordinates are equivalent to planes of the asymmetric unit not belonging to the representation domain. For the parameter ranges see Table 1.5.5.4.

(b) Brillouin zone (thin lines), representation domain (thick lines) and asymmetric unit (dashed lines, partly protruding) imbedded in the Brillouin zone, which is an orthorhombic elongated rhombicuboctahedron. The diagram is drawn for $a^{*2} = 4$, $b^{*2} = 9$, $c^{*2} = 16$, i.e. $a^{*2} + b^{*2} < c^{*2}$. The endpoint of line G is G_0 etc., the free coordinate of G_0 is g_0 etc. Asymmetric unit $\Gamma TZ'YZY'\Gamma T'$ of $Imm2$, IT A, p. 246. The part $\Gamma TZ'YQ_0H_0\Lambda_0G_0$ is common to both bodies; the part $ZY'\Gamma T'\Lambda_0G_0Q_0H_0$ is equivalent to the part of the representation domain with negative z values through a twofold screw rotation 2_1 around the axis $\frac{1}{4}, \frac{1}{4}, z$. Coordinates of the points: $\Gamma = 0, 0, 0 \sim \Gamma' = \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; $Y = 0, \frac{1}{2}, 0 \sim Y' = \frac{1}{2}, 0, \frac{1}{2}$; $Z = 0, 0, \frac{1}{2} \sim Z' = \frac{1}{2}, \frac{1}{2}, 0$; $T = \frac{1}{2}, 0, 0 \sim T' = 0, \frac{1}{2}, \frac{1}{2}$; $\Lambda_0 = 0, 0, \lambda_0 \sim Q_0 = \frac{1}{2}, \frac{1}{2}, q_0$; $G_0 = \frac{1}{2}, 0, g_0 \sim H_0 = 0, \frac{1}{2}, h_0$. The coordinates of the points are $\lambda_0 = 1/4[1 + (a^{*2} + b^{*2})/c^{*2}]$; $q_0 = 1/2 - \lambda_0$; $g_0 = 1/4[1 + (b^{*2} - a^{*2})/c^{*2}]$; $h_0 = 1/2 - g_0$. The sign \sim means symmetrically equivalent. There are no special points. The points $\Gamma, T, Y, Z', \Lambda_0, Q_0, G_0$ and H_0 belong to special lines. The points with negative z coordinates are equivalent to those already listed. Lines: $\Lambda = \Gamma\Lambda_0 = 0, 0, z$; $Q = Z'Q_0 = \frac{1}{2}, \frac{1}{2}, z$; $G = TG_0 = \frac{1}{2}, 0, z$; $H = YH_0 = 0, \frac{1}{2}, z$. The lines $\Sigma = \Gamma T = x, 0, 0$; $C = YZ' = x, \frac{1}{2}, 0$; $\Delta = \Gamma Y = 0, y, 0$; $D = TZ' = \frac{1}{2}, y, 0$; $Q_0G_0, G_0\Lambda_0, \Lambda_0H_0$ and H_0Q_0 have no special symmetry but belong to special planes. The lines $\Gamma\bar{\Lambda}_0, Z'\bar{Q}_0, T\bar{G}_0$ and $Y\bar{H}_0$ of the representation domain to the points $\bar{\Lambda}, \bar{Q}_0, \bar{G}_0$ and \bar{H}_0 with negative z coordinates are equivalent to lines of the asymmetric unit not belonging to the representation domain. Planes: $E = \Gamma YH_0\Lambda_0 = 0, y, z$; $F = TZ'Q_0G_0 = \frac{1}{2}, y, z$; $J = \Gamma\Lambda_0G_0T = x, 0, z$; $K = YH_0Q_0Z' = x, \frac{1}{2}, z$. The planes $x, y, 0$ and $\Lambda_0G_0Q_0H_0$ belong to the general position GP , as does the negative counterpart of $\Lambda_0G_0Q_0H_0$. The planes $\Gamma\bar{\Lambda}_0\bar{G}_0T, \Gamma\bar{\Lambda}_0\bar{H}_0Y, Y\bar{H}_0\bar{Q}_0Z'$ and $T\bar{G}_0\bar{Q}_0Z'$ of the representation domain to the points $\bar{\Lambda}, \bar{Q}_0, \bar{G}_0$ and \bar{H}_0 with negative z coordinates are equivalent to planes of the asymmetric unit not belonging to the representation domain. For the parameter ranges see Table 1.5.5.4.

(c) Brillouin zone (thin lines), representation domain (thick lines) and asymmetric unit (dashed lines, partly protruding) imbedded in the Brillouin zone, which is an orthorhombic elongated rhombicuboctahedron. The diagram is drawn for $a^{*2} = 49$, $b^{*2} = 9$, $c^{*2} = 16$, i.e. $a^{*2} > b^{*2} + c^{*2}$. The endpoint of line A is A_0 etc., the free coordinate of A_0 is a_0 etc. Asymmetric unit $\Gamma TZ'YZY'\Gamma T'$ of $Imm2$, IT A, p. 246. The part $\Gamma\Sigma_0C_0YZA_0U_0T'$ is common to both bodies; the part $\Sigma_0TZ'C_0A_0Y'\Gamma T'U_0$ is equivalent to the part of the representation domain with negative z values through a twofold screw rotation 2_1 around the axis $\frac{1}{4}, \frac{1}{4}, z$. Coordinates of the points: $\Gamma = 0, 0, 0 \sim \Gamma' = \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; $Y = 0, \frac{1}{2}, 0 \sim Y' = \frac{1}{2}, 0, \frac{1}{2}$; $Z = 0, 0, \frac{1}{2} \sim Z' = \frac{1}{2}, \frac{1}{2}, 0$; $T = \frac{1}{2}, 0, 0 \sim T' = 0, \frac{1}{2}, \frac{1}{2}$; $\Sigma_0 = \sigma_0, 0, 0 \sim U_0 = u_0, \frac{1}{2}, \frac{1}{2}$; $A_0 = a_0, 0, \frac{1}{2} \sim C_0 = c_0, \frac{1}{2}, 0$. The coordinates of the points are $\sigma_0 = 1/4[1 + (b^{*2} + c^{*2})/a^{*2}]$; $u_0 = 1/2 - \sigma_0$; $a_0 = 1/4[1 + (b^{*2} - c^{*2})/a^{*2}]$; $c_0 = 1/2 - a_0$. The sign \sim means symmetrically equivalent. There are no special points. The points Γ, Z, Y and T' belong to special lines, Σ_0, U_0, A_0 and C_0 belong to special planes. The points with negative z coordinates are equivalent to those already listed. Lines: $\Lambda = \Gamma Z = 0, 0, z$; $H = YT' = 0, \frac{1}{2}, z$. The lines $\Sigma = \Gamma\Sigma_0 = x, 0, 0$; $U = T'U_0 = x, \frac{1}{2}, \frac{1}{2}$; $A = ZA_0 = x, 0, \frac{1}{2}$; $C = YC_0 = x, \frac{1}{2}, 0$; $\Delta = \Gamma Y = 0, y, 0$; $B = ZT' = 0, y, \frac{1}{2}$; $U_0A_0, A_0\Sigma_0, \Sigma_0C_0$ and C_0U_0 have no special symmetry but belong to special planes. The lines $\Gamma\bar{Z}$ and $Y\bar{T}'$ of the representation domain to the points \bar{Z} and \bar{T}' with negative z coordinates are equivalent to lines of the asymmetric unit not belonging to the representation domain. Planes: $E = \Gamma YT'Z = 0, y, z$; $J = \Gamma\Sigma_0A_0Z = x, 0, z$; $K = YC_0U_0T' = x, \frac{1}{2}, z$. The planes $x, y, 0$; $x, y, \frac{1}{2}$; and $\Sigma_0C_0U_0A_0$ belong to the general position GP , as does the negative counterpart of $\Sigma_0C_0U_0A_0$. The planes $\Gamma\bar{Z}\bar{T}'\bar{Y}, \Gamma\Sigma_0\bar{A}_0\bar{Z}$ and $Y\bar{T}'\bar{U}_0\bar{C}_0$ of the representation domain to the points \bar{Z}, \bar{T}', A_0 and U_0 with negative z coordinates are equivalent to planes of the asymmetric unit not belonging to the representation domain. For the parameter ranges see Table 1.5.5.4.

The fourth possible type of Brillouin zone with $b^{*2} > a^{*2} + c^{*2}$ is similar to that displayed in (c). It can be obtained from this by exchanging a^* and b^* and changing the letters for the points, lines and planes correspondingly.