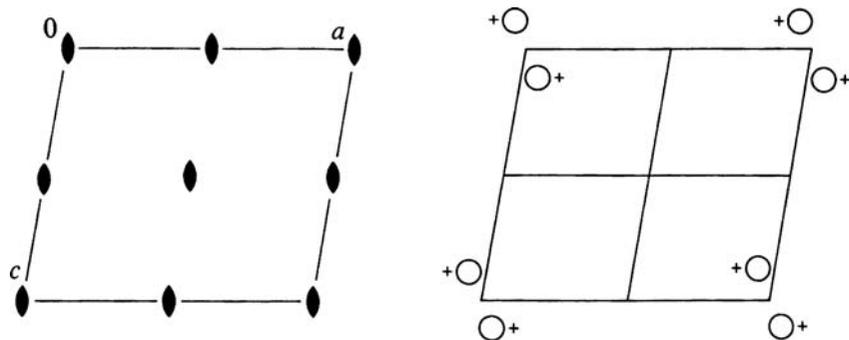# 1. INTRODUCTION TO SPACE-GROUP SYMMETRY

Figure 1.4.2.7
Symmetry-element diagram (left) and general-position diagram (right) for the space group *P*2, No. 3 (unique axis *b*, cell choice 1).

the graphical symbol for a mirror plane is used for its representation on the symmetry-element diagrams of the space groups. For example, the mirror plane $0, y, z$ shown on the symmetry-element diagram of *Fmm*2 (42), *cf.* Fig. 1.4.2.3, represents all glide reflections of the element set of the defining operation $0, y, z$ [symmetry operation (4) of the general-position $(0, 0, 0)+$ set, *cf.* Fig. 1.4.2.2], including the *n*-glide reflection $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ [entry (4) of the general-position $(0, \frac{1}{2}, \frac{1}{2})+$ set]. In a similar way, the graphical symbols of the mirror planes $x, 0, z$ also represent the *n*-glide reflections $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ [entry (3) of the general-position $(\frac{1}{2}, 0, \frac{1}{2})+$ set] of *Fmm*2.

General-position diagram

The graphical presentations of the space-group symmetries provided by the general-position diagrams consist of a set of general-position points which are symmetry equivalent under the symmetry operations of the space group. Starting with a point in the upper left corner of the unit cell, indicated by an open circle with a sign '+', all the displayed points inside and near the unit cell are images of the starting point under some symmetry operation of the space group. Because of the one-to-one correspondence between the image points and the symmetry opera-

tions, the number of general-position points in the unit cell (excluding the points that are equivalent by integer translations) equals the multiplicity of the general position. The coordinates of the points in the projection plane can be read directly from the diagram. For all systems except cubic, only one parameter is necessary to describe the height along the projection direction. For example, if the height of the starting point above the projection plane is indicated by a '+' sign, then signs '+', '−' or their combinations with fractions (*e.g.* $\frac{1}{2}+$, $\frac{1}{2}-$ *etc.*) are used to specify the heights of the image points. A circle divided by a vertical line represents two points with different coordinates along the projection direction but identical coordinates in the projection plane. A comma ',' in the circle indicates an image point obtained by a symmetry operation $W = (W, w)$ of the second kind [*i.e.* with $\det(W) = -1$, *cf.* Section 1.2.2].

Example

The general-position diagram of $P2_1/c$ (unique axis *b*, cell choice 1) is shown in Fig. 1.4.2.6 (right). The open circles indicate the location of the four symmetry-equivalent points of the space group within the unit cell along with additional eight translation-equivalent points to complete the presentation. The circles with a comma inside indicate the image points generated by operations of the second kind – inversions and glide planes in the present case. The fractions and signs close to the circles indicate their heights in units of *b* of the symmetry-equivalent points along the monoclinic axis. For example, $\frac{1}{2}-$ is a shorthand notation for $\frac{1}{2} - y$.

Notes:

(1) The close relation between the symmetry-element and the general-position diagrams is obvious. For example, the points shown on the general-position diagram are images of a general-position point under the action of the space-group symmetry operations displayed by the corresponding symmetry elements on the symmetry-element diagram. With
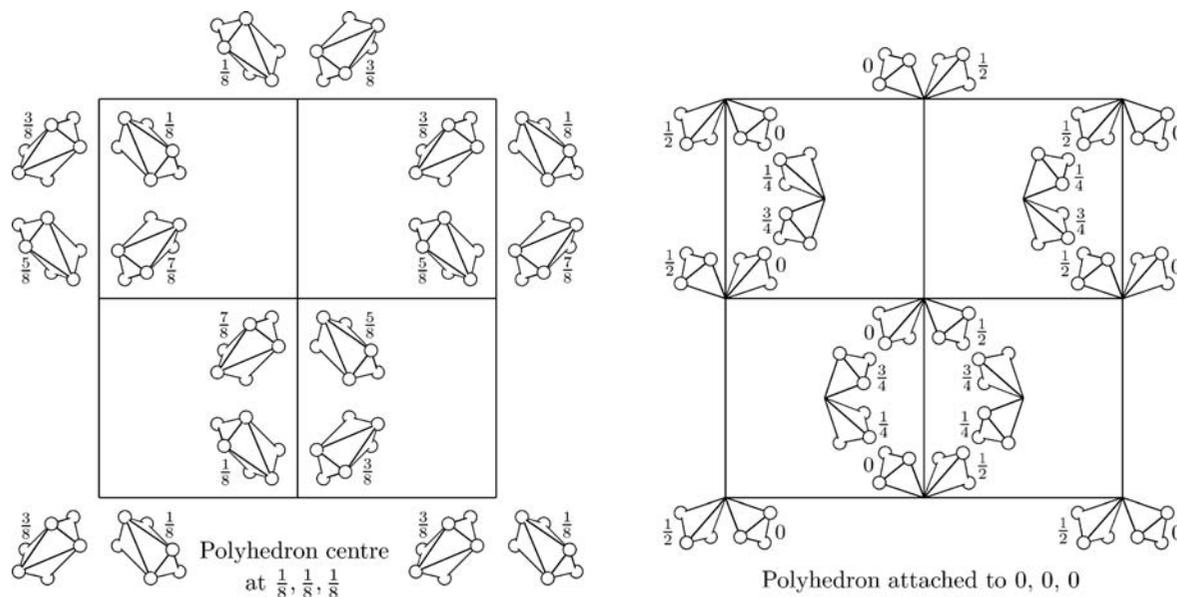
Figure 1.4.2.8
General-position diagrams for the space group $I4_132$ (214). Left: polyhedra (twisted trigonal antiprisms) with centres at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points (site-symmetry group .32). Right: polyhedra (sphenoids) attached to 0, 0, 0 and its equivalent points (site-symmetry group .3.).