particle) in the *h*-cell is related to the 'reference' molecule in the *p*-cell. The known *p*-cell crystallographic symmetry then permits the complete construction of the *p*-cell structure from whatever is the current *h*-cell electron-density representation of the molecule.

The *h*-cell is used to represent the density of a molecule in the standard orientation obtained by averaging all the noncrystallographic units in the *p*-cell. While density within a specific molecule will tend to be reinforced by the averaging procedure, the density outside the molecular boundaries will tend to be diminished. Thus, by averaging into the *h*-cell, the molecular envelope is revealed automatically. Indeed, the greater the NCS, the greater the clarity of the molecular boundary. Hence, the averaged molecule in the *h*-cell can be used to define a molecular mask in the *p*-cell automatically.

Averaging into the *h*-cell is also useful for displaying the molecule in a standard orientation (*i.e.* obtaining the electron-density distribution on skew planes). Thus, it is possible to display the molecule, for instance, with sections perpendicular to a molecular twofold axis, and to position the molecular symmetry axes accurately. From this, it is then easy to define the limits of the molecular asymmetric unit (Fig. 13.4.4.1). Hence, it is possible to save a great deal of computing time by evaluating the electron density in the *h*-cell only at those grid points within and immediately surrounding the noncrystallographic asymmetric unit.

13.4.5. Combining crystallographic and noncrystallographic symmetry

Transformations will now be described which relate noncrystallographically related positions distributed among several fragmented copies of the molecule in the asymmetric unit of the *p*-cell and between the *p*-cell and the *h*-cell.

13.4.5.1. *General considerations*

Let $\mathbf{Y}$ and $\mathbf{X}$ be position vectors in a Cartesian coordinate system whose components have dimensions of length, in the *p*- and *h*-cells, which utilize the same origin as the fractional coordinates, $\mathbf{y}$ and $\mathbf{x}$, respectively. Let $[\beta_p]$ and $[\alpha_h]$ be 'orthogonalization' and 'de-orthogonalization' matrices in the *p*- and *h*-cells, respectively (Rossmann & Blow, 1962). Then

$$\begin{aligned} \mathbf{Y} &= [\beta_p]\mathbf{y} \quad \text{and} \quad \mathbf{x} = [\alpha_h]\mathbf{X}, \\ [\alpha_p] &= [\beta_p]^{-1} \quad \text{and} \quad [\alpha_h] = [\beta_h]^{-1}. \end{aligned} \tag{13.4.5.1}$$

Thus, for instance, $[\alpha_h]$ denotes a matrix that transforms a Cartesian set of unit vectors to fractional distances along the unit-cell vectors $\mathbf{a}_h, \mathbf{b}_h, \mathbf{c}_h$.

Let the Cartesian coordinates $\mathbf{Y}$ and $\mathbf{X}$ be related by the rotation matrix $[\omega]$ and the translation vector $\mathbf{D}$ such that

$$\mathbf{X} = [\omega]\mathbf{Y} + \mathbf{D}. \tag{13.4.5.2}$$

If the molecules are to be averaged among different unit cells, then each *p*-cell must be related to the standard *h*-cell orientation by a different $[\omega]$ and $\mathbf{D}$. Then, from (13.4.5.1) and (13.4.5.2)

$$\mathbf{X} = [\omega][\beta_p]\mathbf{y} + \mathbf{D}. \tag{13.4.5.3}$$

Now, if $[\omega]$ represents the rotational relationship between the 'reference' molecule, $m = 1$, in the *p*-cell with respect to the *h*-cell, then from (13.4.5.3)

$$\mathbf{X} = [\omega][\beta_p]\mathbf{y}_{m=1} + \mathbf{D},$$

where $\mathbf{y}_m$ refers to the fractional coordinates of the *m*th molecule in the *p*-cell.

Assuming there is only one molecule per asymmetric unit in the *p*-cell, let the *m*th molecule in the *p*-cell be related to the reference molecule by the crystallographic rotation $[\mathrm{T}_m]$ and translational operators $\mathbf{t}_m$, such that

$$\mathbf{y}_m = [\mathrm{T}_m]\mathbf{y}_{m=1} + \mathbf{t}_m. \tag{13.4.5.4}$$

For convenience, all translational components will initially be neglected in the further derivations below, but they will be reintroduced in the final stages. Hence, from (13.4.5.3) and (13.4.5.4)

$$\mathbf{X} = \{[\omega][\beta_p][\mathrm{T}_m^{-1}]\}\mathbf{y}_m. \tag{13.4.5.5}$$

Further, if $\mathbf{X}_n$ refers to the *n*th subunit within the molecule in the *h*-cell, and similarly if $\mathbf{y}_{m,n}$ refers to the *n*th subunit within the *m*th molecule of the *p*-cell, then from (13.4.5.5)

$$\mathbf{X}_n = \{[\omega][\beta_p][\mathrm{T}_m^{-1}]\}\mathbf{y}_{m,n}. \tag{13.4.5.6}$$

Finally, the rotation matrix $[\mathrm{R}_n]$ is used to define the relationship among the N ($N = 2$ for a dimer, 4 for a 222 tetramer, 60 for an icosahedral virus *etc.*) noncrystallographic asymmetric units of the molecule within the *h*-cell. Then

$$\mathbf{X}_n = [\mathrm{R}_n]\mathbf{X}_{n=1}. \tag{13.4.5.7}$$

13.4.5.2. *Averaging with the p-cell*

Consider averaging the density at N noncrystallographically related points in the *p*-cell and replacing that density into the *p*-cell. By substituting for $\mathbf{X}_n$ and $\mathbf{X}_{n=1}$ in (13.4.5.7) and using (13.4.5.6),

$$\{[\omega][\beta_p][\mathrm{T}_m^{-1}]\}\mathbf{y}_{m,n} = [\mathrm{R}_n]\{[\omega][\beta_p][\mathrm{T}_m^{-1}]\}\mathbf{y}_{m,n=1},$$

or

$$\mathbf{y}_{m,n} = \{[\omega][\beta_p][\mathrm{T}_m^{-1}]\}^{-1} \times [\mathrm{R}_n]\{[\omega][\beta_p][\mathrm{T}_m^{-1}]\}\mathbf{y}_{m,n=1}. \tag{13.4.5.8}$$

Now set

$$\begin{aligned} [\mathrm{E}_{m,n}] &= \{[\omega][\beta_p][\mathrm{T}_m^{-1}]\}^{-1}[\mathrm{R}_n]\{[\omega][\beta_p][\mathrm{T}_m^{-1}]\} \\ &= [\mathrm{T}_m][\alpha_p][\omega^{-1}][\mathrm{R}_n][\omega][\beta_p][\mathrm{T}_m^{-1}], \end{aligned} \tag{13.4.5.9}$$

giving

$$\mathbf{y}_{m,n} = [\mathrm{E}_{m,n}]\mathbf{y}_{m,n=1} + \mathbf{e}_{m,n}, \tag{13.4.5.10}$$

where $\mathbf{e}_{m,n}$ is the corresponding translational element. Note that multiplication by $[\mathrm{E}_{m,n}]$ thus corresponds to the following sequence of transformations: (1) placing all the crystallographically related subunits into the reference orientation with $[\mathrm{T}_m^{-1}]$; (2) 'orthogonalizing' the coordinates with $[\beta_p]$; (3) rotating the coordinates into the *h*-cell with $[\omega]$; (4) rotating from the reference subunit of the molecule of the *h*-cell with $[\mathrm{R}_n]$; (5) rotating these back into the *p*-cell with $[\omega^{-1}]$; (6) 'de-orthogonalizing' in the *p*-cell with $[\alpha_p]$; and (7) placing these back into each of the M crystallographic asymmetric units of the *p*-cell with $[\mathrm{T}_m]$.

The translational elements, $\mathbf{e}_{m,n}$, can now be evaluated. Let $\mathbf{s}_{p,m}$ be the fractional coordinates of the centre (or some arbitrary position) of the *m*th molecule in the *p*-cell; hence, $\mathbf{s}_{p,m=1}$ denotes the molecular centre position of the reference molecule in the *p*-cell. If $\mathbf{s}_{p,m}$ is at the intersection of the molecular rotation axes, then it will be the same for all *n* molecular asymmetric units. Therefore, it follows from (13.4.5.10) that

$$\mathbf{e}_{m,n} = \mathbf{s}_{p,m} - [\mathrm{E}_{m,n}]\mathbf{s}_{p,m=1}, \tag{13.4.5.11a}$$

or

$$\mathbf{y}_{m,n} = [\mathrm{E}_{m,n}]\mathbf{y}_{m,n=1} + (\mathbf{s}_{p,m} - [\mathrm{E}_{m,n}]\mathbf{s}_{p,m=1}). \tag{13.4.5.11b}$$

Equation (13.4.5.11*b*) can be used to find all the N noncrystallographic asymmetric units within the crystallographic asymmetric

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references