Table 1.4.4.1. *Correspondence between types of centring in direct and reciprocal lattices*

Direct lattice		Reciprocal lattice		
Lattice type(s)	Centring translations	Lattice type(s)	Restriction on *hkl*	Multiple unit cell
P, *R*		*P*, *R*		$\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$
A	$0, \frac{1}{2}, \frac{1}{2}$	*A*	$k+l=2n$	$\mathbf{a}^*$, $2\mathbf{b}^*$, $2\mathbf{c}^*$
B	$\frac{1}{2}, 0, \frac{1}{2}$	*B*	$h+l=2n$	$2\mathbf{a}^*$, $\mathbf{b}^*$, $2\mathbf{c}^*$
C	$\frac{1}{2}, \frac{1}{2}, 0$	*C*	$h+k=2n$	$2\mathbf{a}^*$, $2\mathbf{b}^*$, $\mathbf{c}^*$
I	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	*F*	$h+k+l=2n$	$2\mathbf{a}^*$, $2\mathbf{b}^*$, $2\mathbf{c}^*$
F	$0, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$	*I*	$k+l=2n$ $h+l=2n$ $h+k=2n$	$2\mathbf{a}^*$, $2\mathbf{b}^*$, $2\mathbf{c}^*$
$R_{\rm hex}$	$\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$	$R_{\rm hex}$	$-h+k+l=3n$	$3\mathbf{a}^*$, $3\mathbf{b}^*$, $3\mathbf{c}^*$

Following Bienenstock & Ewald, the operators $(\boldsymbol{P}, -\mathbf{t})$ are symmetry operators that act on the positions $[\mathbf{h}^T : 0]$ in Fourier space, provided they satisfy the following requirements: (i) the application of such an operator leaves the magnitude of the (generally) complex Fourier coefficient unchanged, and (ii) after g successive applications of an operator, where g is the order of its rotation part, the phase remains unchanged up to a shift by an integer multiple of 2π (a trivial phase shift, corresponding to a translation by a lattice vector in direct space).

If our function is the electron density in the crystal, the first requirement is obviously satisfied since $|F(\mathbf{h})| = |F(\mathbf{h}^T\boldsymbol{P})|$, where F is the structure factor [*cf.* equation (1.4.2.4)]. In order to make use of the second requirement in deriving permissible symmetry operators on Fourier space, all the relevant transformations, *i.e.* those which have rotation operators of the orders 1, 2, 3, 4 and 6, must be individually examined. A comprehensive example, covering most of the tetragonal system, can be found in Bienenstock & Ewald (1962).

It is of interest to illustrate the above process for a simple particular instance. Consider an operation, the rotation part of which involves a mirror plane, and assume that it is associated with the monoclinic system, in the second setting (unique axis b). We denote the operator by $(\boldsymbol{m}, -\mathbf{u})$, where $\mathbf{u}^T = (uvw)$, and the permissible values of u, v and w are to be determined. The operation is of order 2, and according to requirement (ii) above we have to evaluate

$$\begin{aligned}[\mathbf{h}^T : 0](\boldsymbol{m}, -\mathbf{u})^2 &= [\mathbf{h}^T : 0](\boldsymbol{I}, -\boldsymbol{m}\mathbf{u} - \mathbf{u}) \\ &= [\mathbf{h}^T : -\mathbf{h}^T(\boldsymbol{m} + \boldsymbol{I})\mathbf{u}] \\ &= [hkl : -2(hu + lw)], \end{aligned} \tag{1.4.4.13}$$

where

$$\boldsymbol{m} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

is the matrix representing the operation of reflection and $\boldsymbol{I}$ is the unit matrix. For $(\boldsymbol{m}, -\mathbf{u})$ to be an admissible symmetry operator, the phase-shift part of (1.4.4.13), *i.e.* $-2(hu + lw)$, must be an integer (multiple of 2π). The smallest non-negative values of u and w which satisfy this are the pairs: $u = w = 0$, $u = \frac{1}{2}$ and $w = 0$, $u = 0$ and $w = \frac{1}{2}$, and $u = w = \frac{1}{2}$. We have thus obtained four symmetry operators in Fourier space, which are identical (except for the sign of their translational parts) to those of the direct-space monoclinic mirror and glide-plane operations. The fact that the component v cancels out simply means that an arbitrary component of the phase shift can be added along the b^* axis; this is concurrent with arbitrary direct-space translations that appear in the characterization of individual types of space-group operations [see *e.g.* Koch & Fischer (2005)].

Each of the 230 space groups, which leaves invariant a (real and non-negative) function with the periodicity of the crystal, thus has its counterpart which determines the symmetry of the Fourier expansion coefficients of this function, with equivalent positions given in Table A1.4.4.1.

1.4.4.5. Relationships between direct and reciprocal Bravais lattices

Centred Bravais lattices in crystal space give rise to systematic absences of certain classes of reflections (*IT* I, 1952; *IT* A, 1983) and the corresponding points in the reciprocal lattice have accordingly zero weights. These absences are periodic in reciprocal space and their 'removal' from the reciprocal lattice results in a lattice which – like the direct one – must belong to one of the fourteen Bravais lattice types. This must be so since the point group of a crystal leaves its lattice – and also the associated reciprocal lattice – unchanged. The magnitudes of the structure factors (the weight functions) are also invariant under the operation of this point group.

The correspondence between the types of centring in direct and reciprocal lattices is given in Table 1.4.4.1.

Notes:

(i) The vectors $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$, appearing in the definition of the multiple unit cell in the reciprocal lattice, define this lattice *prior to the removal* of lattice points with zero weights (absences). All the restrictions on *hkl* pertain to indexing on $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$.

(ii) The centring type of the reciprocal lattice refers to the multiple unit cell given in the table.

(iii) The centring type denoted by $R_{\rm hex}$ is a representation of the rhombohedral lattice R by a triple hexagonal unit cell, in the obverse setting (*IT* I, 1952), *i.e.* according to the transformation

$$\begin{aligned} \mathbf{a} &= \mathbf{a}_R - \mathbf{b}_R \\ \mathbf{b} &= \mathbf{b}_R - \mathbf{c}_R \\ \mathbf{c} &= \mathbf{a}_R + \mathbf{b}_R + \mathbf{c}_R, \end{aligned} \tag{1.4.4.14}$$

where $\mathbf{a}_R$, $\mathbf{b}_R$ and $\mathbf{c}_R$ pertain to a primitive unit cell in the rhombohedral lattice R.

The corresponding multiple reciprocal cell, with centring denoted by $R_{\rm hex}$, contains nine lattice points with coordinates 000, 021, 012, 101, 202, 110, 220, 211 and 122 – indexed on the usual reciprocal to the triple hexagonal unit cell defined by (1.4.4.14). Detailed derivations of these correspondences are given by Buerger (1942), and an elementary proof of the reciprocity of I and F lattices can be found, *e.g.*, in pamphlet No. 4 of the Commission on Crystallographic Teaching (Authier, 1981).