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).

Intuitive proofs follow directly from the restrictions on *hkl*, given in Table 1.4.4.1.

APPENDIX A1.4.1
Comments on the preparation and usage of the tables

By U. Shmueli

The straightforward but rather extensive calculations and text processing related to Tables A1.4.3.1 through A1.4.3.7 and Table A1.4.4.1 in Appendices 1.4.3 and 1.4.4, respectively, were performed with the aid of a combination of FORTRAN and REDUCE (Hearn, 1973) programs, designed so as to enable the author to produce the table entries directly from a space-group symbol and with a minimum amount of intermediate manual intervention. The first stage of the calculation, the generation of a space group (coordinates of the equivalent positions), was accomplished with the program *SPGRGEN*, the algorithm of which was described in some detail elsewhere (Shmueli, 1984). A complete list of computer-adapted space-group symbols, processed by *SPGRGEN* and not given in the latter reference, is presented in Table A1.4.2.1 of Appendix 1.4.2.

The generation of the space group is followed by a construction of symbolic expressions for the scalar products $\mathbf{h}^T(\boldsymbol{P}\mathbf{r}+\mathbf{t})$; *e.g.* for position No. (13) in the space group $P4_132$ (No. 213, *IT* I, 1952, *IT* A, 1983), this scalar product is given by $h(\frac{3}{4}+y)+k(\frac{1}{4}+x)+l(\frac{1}{4}-z)$. The construction of the various table entries consists of expanding the sines and cosines of these scalar products, performing the required summations, and simplifying the result where possible. The construction of the scalar products in a FORTRAN program is fairly easy and the extremely tedious trigonometric calculations required by equations (1.4.2.19) and (1.4.2.20) can be readily performed with the aid of one of several available computer-algebraic languages (for a review, see *Computers in the New Laboratory – a Nature Survey*, 1981); the REDUCE language was employed for the above purpose.

Since the REDUCE programs required for the summations in (1.4.2.19) and (1.4.2.20) for the various space groups were seen to have much in common, it was decided to construct a FORTRAN interface which would process the space-group input and prepare automatically REDUCE programs for the algebraic work. The least straightforward problem encountered during this work was the need to 'convince' the interface to generate *hkl* parity assignments which are appropriate to the space-group information input. This was solved for all the crystal families except the hexagonal by setting up a 'basis' of the form: $h/2, k/2, l/2, (k+l)/2, \ldots, (h+k+l)/4$ and representing the translation parts of the scalar products, $\mathbf{h}^T\mathbf{t}$, as sums of such 'basis functions'. A subsequent construction of an automatic parity routine proved to be easy and the interface could thus produce any number of REDUCE programs for the summations in (1.4.2.19) and (1.4.2.20) using a list of space-group symbols as the sole input. These included trigonal and hexagonal space groups with translation components of $\frac{1}{2}$. This approach seemed to be too awkward for some space groups containing threefold and sixfold screw axes, and these were treated individually.

There is little to say about the REDUCE programs, except that the output they generate is at the same level of trigonometric complexity as the expressions for A and B appearing in Volume I (*IT* I, 1952). This could have been improved by making use of the pattern-matching capabilities that are incorporated in REDUCE, but it was found more convenient to construct a FORTRAN interpreter which would detect in the REDUCE output the basic building blocks of the trigonometric structure factors (see Section 1.4.3.3) and perform the required transformations.

Tables A1.4.3.1–A1.4.3.7 were thus constructed with the aid of a chain composed of (i) a space-group generating routine, (ii) a FORTRAN interface, which processes the space-group input and 'writes' a complete REDUCE program, (iii) execution of the REDUCE program and (iv) a FORTRAN interpreter of the REDUCE output in terms of the abbreviated symbols to be used in the tables. The computation was at a 'one-group-at-a-time' basis and the automation of its repetition was performed by means of procedural constructs at the operating-system level. The construction of Table A1.4.4.1 involved only the preliminary stage of the processing of the space-group information by the FORTRAN interface. All the computations were carried out on a Cyber 170–855 at the Tel Aviv University Computation Center.

It is of some importance to comment on the recommended usage of the tables included in this chapter in automatic computations. If, for example, we wish to compute the expression: $A=-8(\mathrm{Escs}+\mathrm{Ossc})$, use can be made of the facility provided by most versions of FORTRAN of transferring subprogram names as parameters of a FUNCTION. We thus need only two FUNCTIONs for any calculation of A and B for a cubic space group, one FUNCTION for the block of even permutations of x, y and z:

```
      FUNCTION E(P,Q,R)
      EXTERNAL SIN,COS
      COMMON/TSF/TPH,TPK,TPL,X,Y,Z
      E = P(TPH * X) * Q(TPK * Y) * R(TPL * Z)
     1 + P(TPH * Z) * Q(TPK * X) * R(TPL * Y)
     2 + P(TPH * Y) * Q(TPK * Z) * R(TPL * X)
      RETURN
      END
```

where TPH, TPK and TPL denote $2\pi h$, $2\pi k$ and $2\pi l$, respectively, and a similar FUNCTION, say O(P,Q,R), for the block of odd permutations of x, y and z. The calling statement in the calling (sub)program can thus be:

```
A = -8 * (E(SIN,COS,SIN) + O(SIN,SIN,COS)).
```

A small number of such FUNCTIONs suffices for all the space-group-specific computations that involve trigonometric structure factors.

APPENDIX A1.4.2
Space-group symbols for numeric and symbolic computations

A1.4.2.1. Introduction

By U. Shmueli, S. R. Hall and R. W. Grosse-Kunstleve

This appendix lists two sets of computer-adapted space-group symbols which are implemented in existing crystallographic software and can be employed in the automated generation of space-group representations. The computer generation of space-group symmetry information is of well known importance in many crystallographic calculations, numeric as well as symbolic. A prerequisite for a computer program that generates this information is a set of computer-adapted space-group symbols which are based on the generating elements of the space group to be derived. The sets of symbols to be presented are: