of the distinct orbits for the action of G in X may be obtained in the form

$$D_k = X_1 \times \ldots \times X_{k-1} \times \{x_{i_k}^{(k)}\}_{i_k \in I_k} \times X_{k+1} \times \ldots \times X_n$$

for each $k = 1, 2, \ldots, n$, *i.e.* by taking a fundamental domain in X_k and all the elements in X_j with $j \neq k$. The action of G on each D_k does indeed generate the whole of X: given an arbitrary element $y = (y_1, y_2, \ldots, y_n)$ of X, there is an index $i_k \in I_k$ such that $y_k \in Gx_{i_k}^{(k)}$ and a coset of $G_{x_{i_k}^{(k)}}$ in G such that $y_k = \gamma x_{i_k}^{(k)}$ for any representative γ of that coset; then

$$y = \gamma(\gamma^{-1}y_1, \ldots, \gamma^{-1}y_{k-1}, x_{i_k}^{(k)}, \gamma^{-1}y_{k+1}, \ldots, \gamma^{-1}y_n)$$

which is of the form $y = \gamma d_k$ with $d_k \in D_k$.

The various D_k are related in a simple manner by 'transposition' or 'orbit exchange' (the latter name is due to J. W. Cooley). For instance, D_j may be obtained from $D_k (j \neq k)$ as follows: for each $y_j \in X_j$ there exists $g(y_j) \in G$ and $i_j(y_j) \in I_j$ such that $y_j = g(y_j)x_{i_j(y_j)}^{(j)}$; therefore

$$D_j = \bigcup_{y_j \in X_j} [g(y_j)]^{-1} D_k,$$

since the fundamental domain of X_k is thus expanded to the whole of X_k, while X_j is reduced to its fundamental domain. In other words: orbits are simultaneously collapsed in the jth factor and expanded in the kth.

When G operates without fixed points in each X_k (*i.e.* $G_{x_k} = \{e\}$ for all $x_k \in X_k$), then each D_k is a fundamental domain for the action of G in X. The existence of fixed points in some or all of the X_k complicates the situation in that for each k and each $x_k \in X_k$ such that $G_{x_k} \neq \{e\}$ the action of G/G_{x_k} on the other factors must be examined. Shenefelt (1988) has made a systematic study of orbit exchange for space group $P622$ and its subgroups.

Orbit exchange will be encountered, in a great diversity of forms, as the basic mechanism by which intermediate results may be rearranged between the successive stages of the computation of crystallographic Fourier transforms (Section 1.3.4.3).

1.3.4.2.2.3. *Classification of crystallographic groups*

Let Γ be a crystallographic group, Λ the normal subgroup of its lattice translations, and G the finite factor group Γ/Λ. Then G acts on Λ by conjugation [Section 1.3.4.2.2.2(*d*)] and this action, being a mapping of a lattice into itself, is representable by matrices with integer entries.

The classification of crystallographic groups proceeds from this observation in the following three steps:

Step 1: find all possible finite abstract groups G which can be represented by 3×3 integer matrices.

Step 2: for each such G find all its inequivalent representations by 3×3 integer matrices, equivalence being defined by a change of primitive lattice basis (*i.e.* conjugation by a 3×3 integer matrix with determinant ± 1).

Step 3: for each G and each equivalence class of integral representations of G, find all inequivalent extensions of the action of G from Λ to $T(3)$, equivalence being defined by an affine coordinate change [*i.e.* conjugation by an element of $A(3)$].

Step 1 leads to the following groups, listed in association with the crystal system to which they later give rise:

$\mathbb{Z}/2\mathbb{Z}$	monoclinic
$\mathbb{Z}/2\mathbb{Z} \oplus \mathbb{Z}/2\mathbb{Z}$	orthorhombic
$\mathbb{Z}/3\mathbb{Z}, (\mathbb{Z}/3\mathbb{Z}) \rtimes \{\alpha\}$	trigonal
$\mathbb{Z}/4\mathbb{Z}, (\mathbb{Z}/4\mathbb{Z}) \rtimes \{\alpha\}$	tetragonal
$\mathbb{Z}/6\mathbb{Z}, (\mathbb{Z}/6\mathbb{Z}) \rtimes \{\alpha\}$	hexagonal
$(\mathbb{Z}/2\mathbb{Z} \oplus \mathbb{Z}/2\mathbb{Z}) \rtimes \{S_3\}$	cubic

and the extension of these groups by a centre of inversion. In this list $\rtimes$ denotes a semi-direct product [Section 1.3.4.2.2.2(*d*)], α denotes the automorphism $g \longmapsto g^{-1}$, and S_3 (the group of permutations on three letters) operates by permuting the copies of $\mathbb{Z}/2\mathbb{Z}$ (using the subgroup A_3 of cyclic permutations gives the tetrahedral subsystem).

Step 2 leads to a list of 73 equivalence classes called *arithmetic classes* of representations $g \longmapsto \mathbf{R}_g$, where $\mathbf{R}_g$ is a 3×3 integer matrix, with $\mathbf{R}_{g_1 g_2} = \mathbf{R}_{g_1}\mathbf{R}_{g_2}$ and $\mathbf{R}_e = \mathbf{I}_3$. This enumeration is more familiar if equivalence is relaxed so as to allow conjugation by *rational* 3×3 matrices with determinant ± 1: this leads to the 32 crystal classes. The difference between an arithmetic class and its rational class resides in the choice of a lattice mode (P, $A/B/C$, I, F or R). Arithmetic classes always refer to a primitive lattice, but may use inequivalent integral representations for a given geometric symmetry element; while crystallographers prefer to change over to a non-primitive lattice, if necessary, in order to preserve the same integral representation for a given geometric symmetry element. The matrices $\mathbf{P}$ and $\mathbf{Q} = \mathbf{P}^{-1}$ describing the changes of basis between primitive and centred lattices are listed in Table 5.1 and illustrated in Figs. 5.3 to 5.9, pp. 76–79, of Volume A of *International Tables* (Arnold, 1995).

Step 3 gives rise to a system of congruences for the systems of non-primitive translations $\{\mathbf{t}_g\}_{g \in G}$ which may be associated to the matrices $\{\mathbf{R}_g\}_{g \in G}$ of a given arithmetic class, namely:

$$\mathbf{t}_{g_1 g_2} \equiv \mathbf{R}_{g_1}\mathbf{t}_{g_2} + \mathbf{t}_{g_1} \bmod \Lambda,$$

first derived by Frobenius (1911). If equivalence under the action of $A(3)$ is taken into account, 219 classes are found. If equivalence is defined with respect to the action of the subgroup $A^+(3)$ of $A(3)$ consisting only of transformations with determinant +1, then 230 classes called *space-group types* are obtained. In particular, associating to each of the 73 arithmetic classes a trivial set of non-primitive translations ($\mathbf{t}_g = \mathbf{0}$ for all $g \in G$) yields the 73 symmorphic space groups. This third step may also be treated as an abstract problem concerning group extensions, using cohomological methods [Ascher & Janner (1965); see Janssen (1973) for a summary]; the connection with Frobenius's approach, as generalized by Zassenhaus (1948), is examined in Ascher & Janner (1968).

The finiteness of the number of space-group types in dimension 3 was shown by Bieberbach (1912) to be the case in arbitrary dimension. The reader interested in N-dimensional space-group theory for $N > 3$ may consult Brown (1969), Brown *et al.* (1978), Schwarzenberger (1980), and Engel (1986). The standard reference for integral representation theory is Curtis & Reiner (1962).

All three-dimensional space groups G have the property of being *solvable*, *i.e.* that there exists a chain of subgroups

$$G = G_r > G_{r-1} > \ldots > G_1 > G_0 = \{e\},$$

where each G_{i-1} is a normal subgroup of G_1 and the factor group G_i/G_{i-1} is a *cyclic* group of some order m_i $(1 \leq i \leq r)$. This property may be established by inspection, or deduced from a famous theorem of Burnside [see Burnside (1911), pp. 322–323] according to which any group G such that $|G| = p^\alpha q^\beta$, with p and q distinct primes, is solvable; in the case at hand, $p = 2$ and $q = 3$.

The whole classification of 3D space groups can be performed swiftly by a judicious use of the solvability property (L. Auslander, personal communication).

Solvability facilitates the indexing of elements of G in terms of generators and relations (Coxeter & Moser, 1972; Magnus *et al.*, 1976) for the purpose of calculation. By definition of solvability, elements $g_1, g_2, \ldots, g_r$ may be chosen in such a way that the cyclic factor group G_i/G_{i-1} is generated by the coset g_iG_{i-1}. The set $\{g_1, g_2, \ldots, g_r\}$ is then a system of generators for G such that the defining relations [see Brown *et al.* (1978), pp. 26–27] have the particularly simple form

$$\begin{aligned} g_1^{m_1} &= e, \\ g_i^{m_i} &= g_{i-1}^{a(i,\,i-1)} g_{i-2}^{a(i,\,i-2)} \cdots g_1^{a(i,\,1)} \qquad \text{for } 2 \le i \le r, \\ g_i^{-1} g_j^{-1} g_i g_j &= g_{j-1}^{b(i,j,j-1)} g_{j-2}^{b(i,j,j-2)} \cdots g_1^{b(i,j,\,1)} \quad \text{for } 1 \le i < j \le r, \end{aligned}$$

with $0 \le a(i,h) < m_h$ and $0 \le b(i,j,h) < m_h$. Each element g of G may then be obtained uniquely as an 'ordered word':

$$g = g_r^{k_r} g_{r-1}^{k_{r-1}} \cdots g_1^{k_1},$$

with $0 \le k_i < m_i$ for all $i = 1, \ldots, r$, using the algorithm of Jürgensen (1970). Such generating sets and defining relations are tabulated in Brown *et al.* (1978, pp. 61–76). An alternative list is given in Janssen (1973, Table 4.3, pp. 121–123, and Appendix D, pp. 262–271).

1.3.4.2.2.4. *Crystallographic group action in real space*

The action of a crystallographic group Γ may be written in terms of standard coordinates in $\mathbb{R}^3/\mathbb{Z}^3$ as

$$(g, \mathbf{x}) \longmapsto S_g(\mathbf{x}) = \mathbf{R}_g\mathbf{x} + \mathbf{t}_g \bmod \Lambda, \quad g \in G,$$

with

$$S_{g_1g_2} = S_{g_1} S_{g_2}.$$

An important characteristic of the representation $\theta : g \longmapsto S_g$ is its *reducibility*, *i.e.* whether or not it has invariant subspaces other than $\{\mathbf{0}\}$ and the whole of $\mathbb{R}^3/\mathbb{Z}^3$. For triclinic, monoclinic and orthorhombic space groups, θ is reducible to a direct sum of three one-dimensional representations:

$$\mathbf{R}_g = \begin{pmatrix} \mathbf{R}_g^{(1)} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_g^{(2)} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{R}_g^{(3)} \end{pmatrix};$$

for trigonal, tetragonal and hexagonal groups, it is reducible to a direct sum of two representations, of dimension 2 and 1, respectively; while for tetrahedral and cubic groups, it is irreducible.

By Schur's lemma (see *e.g.* Ledermann, 1987), any matrix which commutes with all the matrices $\mathbf{R}_g$ for $g \in G$ must be a scalar multiple of the identity in each invariant subspace.

In the reducible cases, the reductions involve changes of basis which will be *rational*, not integral, for those arithmetic classes corresponding to non-primitive lattices. Thus the simplification of having maximally reduced representation has as its counterpart the use of non-primitive lattices.

The notions of orbit, isotropy subgroup and fundamental domain (or asymmetric unit) for the action of G on $\mathbb{R}^3/\mathbb{Z}^3$ are inherited directly from the general setting of Section 1.3.4.2.2.2. Points $\mathbf{x}$ for which $G_\mathbf{x} \neq \{e\}$ are called *special positions*, and the various types of isotropy subgroups which may be encountered in crystallographic groups have been labelled by means of Wyckoff symbols. The representation operators $S_g^\#$ in $L(\mathbb{R}^3/\mathbb{Z}^3)$ have the form:

$$[S_g^\# f](\mathbf{x}) = f[S_g^{-1}(\mathbf{x})] = f[\mathbf{R}_g^{-1}(\mathbf{x} - \mathbf{t}_g)].$$

The operators $R_g^\#$ associated to the purely rotational part of each transformation S_g will also be used. Note the relation: $S_g^\# = \tau_{\mathbf{t}_g} R_g^\#$.

Let a crystal structure be described by the list of the atoms in its unit cell, indexed by $k \in K$. Let the electron-density distribution about the centre of mass of atom k be described by $\wp_k$ with respect to the standard coordinates $\mathbf{x}$. Then the motif $\wp^0$ may be written as a sum of translates:

$$\wp^0 = \sum_{k \in K} \tau_{\mathbf{x}_k} \wp_k$$

and the crystal electron density is $\wp = r^* \wp^0$.

Suppose that $\wp$ is invariant under Γ. If $\mathbf{x}_{k_1}$ and $\mathbf{x}_{k_2}$ are in the same orbit, say $\mathbf{x}_{k_2} = S_g(\mathbf{x}_{k_1})$, then

$$\tau_{\mathbf{x}_{k_2}} \wp_{k_2} = S_g^\#(\tau_{\mathbf{x}_{k_1}} \wp_{k_1}).$$

Therefore if $\mathbf{x}_k$ is a special position and thus $G_{\mathbf{x}_k} \neq \{e\}$, then

$$S_g^\#(\tau_{\mathbf{x}_k} \wp_k) = \tau_{\mathbf{x}_k} \wp_k \quad \text{for all } g \in G_{\mathbf{x}_k}.$$

This identity implies that

$$\mathbf{R}_g\mathbf{x}_k + \mathbf{t}_g \equiv \mathbf{x}_k \bmod \Lambda$$

(the special position condition), and that

$$\wp_k = R_g^\# \wp_k,$$

i.e. that $\wp_k$ must be invariant by the pure rotational part of $G_{\mathbf{x}_k}$. Trueblood (1956) investigated the consequences of this invariance on the thermal vibration tensor of an atom in a special position (see Section 1.3.4.2.2.6 below).

Let J be a subset of K such that $\{\mathbf{x}_j\}_{j \in J}$ contains exactly one atom from each orbit. An orbit decomposition yields an expression for $\wp^0$ in terms of symmetry-unique atoms:

$$\wp^0 = \sum_{j \in J} \left(\sum_{\gamma_j \in G/G_{\mathbf{x}_j}} S_{\gamma_j}^\#(\tau_{\mathbf{x}_j} \wp_j) \right)$$

or equivalently

$$\wp^0(\mathbf{x}) = \sum_{j \in J} \left\{ \sum_{\gamma_j \in G/G_{\mathbf{x}_j}} \wp_j[\mathbf{R}_{\gamma_j}^{-1}(\mathbf{x} - \mathbf{t}_{\gamma_j}) - \mathbf{x}_j] \right\}.$$

If the atoms are assumed to be Gaussian, write

$$\rho_j(\mathbf{X}) = \frac{Z_j}{|\det \pi \mathbf{U}_j|^{1/2}} \times \exp(-\tfrac{1}{2}\mathbf{X}^T \mathbf{U}_j^{-1} \mathbf{X}) \text{ in Cartesian Å coordinates,}$$

where Z_j is the total number of electrons, and where the matrix $\mathbf{U}_j$ combines the Gaussian spread of the electrons in atom j at rest with the covariance matrix of the random positional fluctuations of atom j caused by thermal agitation.

In crystallographic coordinates:

$$\wp_j(\mathbf{x}) = \frac{Z_j}{|\det \pi \mathbf{Q}_j|^{1/2}} \times \exp(-\tfrac{1}{2}\mathbf{x}^T \mathbf{Q}_j^{-1} \mathbf{x}) \text{ with } \mathbf{Q}_j = \mathbf{A}^{-1}\mathbf{U}_j(\mathbf{A}^{-1})^T.$$

If atom k is in a special position $\mathbf{x}_k$, then the matrix $\mathbf{Q}_k$ must satisfy the identity

$$\mathbf{R}_g \mathbf{Q}_k \mathbf{R}_g^{-1} = \mathbf{Q}_k$$

references