The ability of a given factoring method to accommodate crystallographic symmetry will thus be determined by the extent to which the crystallographic group action respects (or fails to respect) the partitioning of the index set into the substructures pertaining to that method. This remark justifies trying to gain an overall view of the algebraic structures involved, and of the possibilities of a crystallographic group acting 'naturally' on them.

The index sets $\{\mathbf{m}|\mathbf{m}\in\mathbb{Z}^3/\mathbf{N}\mathbb{Z}^3\}$ and $\{\mathbf{h}|\mathbf{h}\in\mathbb{Z}^3/\mathbf{N}^T\mathbb{Z}^3\}$ are finite Abelian groups under component-wise addition. If an iterated addition is viewed as an action of an integer scalar $n\in\mathbb{Z}$ *via*

$$\begin{aligned} n\mathbf{h} &= \mathbf{h}+\mathbf{h}+\ldots+\mathbf{h} \quad (n \text{ times}) && \text{for } n>0,\\ &= \mathbf{0} && \text{for } n=0,\\ &= -(\mathbf{h}+\mathbf{h}+\ldots+\mathbf{h}) \quad (|n| \text{ times}) && \text{for } n<0, \end{aligned}$$

then an Abelian group becomes a *module* over the ring $\mathbb{Z}$ (or, for short, a $\mathbb{Z}$-module), a module being analogous to a vector space but with scalars drawn from a ring rather than a field. The left actions of a crystallographic group G by

$$g: \quad \mathbf{m}\longmapsto \mathbf{R}_g\mathbf{m}+\mathbf{N}\mathbf{t}_g \mod \mathbf{N}\mathbb{Z}^3$$

and by

$$g: \quad \mathbf{h}\longmapsto (\mathbf{R}_g^{-1})^T\mathbf{h} \mod \mathbf{N}^T\mathbb{Z}^3$$

can be combined with this $\mathbb{Z}$ action as follows:

$$\begin{aligned} \textstyle\sum_{g\in G} n_g g: &\quad \mathbf{m}\longmapsto \textstyle\sum_{g\in G} n_g(\mathbf{R}_g\mathbf{m}+\mathbf{N}\mathbf{t}_g) && \mod \mathbf{N}\mathbb{Z}^3,\\ \textstyle\sum_{g\in G} n_g g: &\quad \mathbf{h}\longmapsto \textstyle\sum_{g\in G} n_g[(\mathbf{R}_g^{-1})^T\mathbf{h}] && \mod \mathbf{N}^T\mathbb{Z}^3. \end{aligned}$$

This provides a left action, on the indexing sets, of the set

$$\mathbb{Z}G=\left\{\sum_{g\in G} n_g g \,\middle|\, n_g\in\mathbb{Z} \text{ for each } g\in G\right\}$$

of symbolic linear combinations of elements of G with integral coefficients. If addition and multiplication are defined in $\mathbb{Z}G$ by

$$\left(\sum_{g_1\in G} a_{g_1}g_1\right)+\left(\sum_{g_2\in G} b_{g_2}g_2\right)=\sum_{g\in G}(a_g+b_g)g$$

and

$$\left(\sum_{g_1\in G} a_{g_1}g_1\right)\times\left(\sum_{g_2\in G} b_{g_2}g_2\right)=\sum_{g\in G} c_g g,$$

with

$$c_g=\sum_{g'\in G} a_{g'}b_{(g')^{-1}g},$$

then $\mathbb{Z}G$ is a *ring*, and the action defined above makes the indexing sets into $\mathbb{Z}G$-*modules*. The ring $\mathbb{Z}G$ is called the *integral group ring* of G (Curtis & Reiner, 1962, p. 44).

From the algebraic standpoint, therefore, the interaction between symmetry and factorization can be expected to be favourable whenever the indexing sets of partial transforms are $\mathbb{Z}G$-submodules of the main $\mathbb{Z}G$-modules.

1.3.4.3.4.1. *Multidimensional Cooley–Tukey factorization*

Suppose, as in Section 1.3.3.3.2.1, that the decimation matrix $\mathbf{N}$ may be factored as $\mathbf{N}_1\mathbf{N}_2$. Then any grid point index $\mathbf{m}\in\mathbb{Z}^3/\mathbf{N}\mathbb{Z}^3$ in real space may be written

$$\mathbf{m}=\mathbf{m}_1+\mathbf{N}_1\mathbf{m}_2$$

with $\mathbf{m}_1\in\mathbb{Z}^3/\mathbf{N}_1\mathbb{Z}^3$ and $\mathbf{m}_2\in\mathbb{Z}^3/\mathbf{N}_2\mathbb{Z}^3$ determined by

$$\begin{aligned} \mathbf{m}_1 &= \mathbf{m} && \mod \mathbf{N}_1\mathbb{Z}^3,\\ \mathbf{m}_2 &= \mathbf{N}_1^{-1}(\mathbf{m}-\mathbf{m}_1) && \mod \mathbf{N}_2\mathbb{Z}^3. \end{aligned}$$

These relations establish a one-to-one correspondence $\mathbf{m}\leftrightarrow(\mathbf{m}_1,\mathbf{m}_2)$ between $I=\mathbb{Z}^3/\mathbf{N}\mathbb{Z}^3$ and the Cartesian product $I_1\times I_2$ of $I_1=\mathbb{Z}^3/\mathbf{N}_1\mathbb{Z}^3$ and $I_2=\mathbb{Z}^3/\mathbf{N}_2\mathbb{Z}^3$, and hence $I\cong I_1\times I_2$ as a set. However $I\ncong I_1\times I_2$ as an Abelian group, since in general $\mathbf{m}+\mathbf{m}'\not\leftrightarrow(\mathbf{m}_1+\mathbf{m}_1',\mathbf{m}_2+\mathbf{m}_2')$ because there can be a 'carry' from the addition of the first components into the second components; therefore, $I\ncong I_1\times I_2$ as a $\mathbb{Z}G$-module, which shows that the incorporation of symmetry into the Cooley–Tukey algorithm is not a trivial matter.

Let $g\in G$ act on I through

$$g: \quad \mathbf{m}\longmapsto S_g(\mathbf{m})=\mathbf{R}_g\mathbf{m}+\mathbf{N}\mathbf{t}_g \mod \mathbf{N}\mathbb{Z}^3$$

and suppose that $\mathbf{N}$ 'integerizes' all the non-primitive translations $\mathbf{t}_g$ so that we may write

$$\mathbf{N}\mathbf{t}_g=\mathbf{t}_g^{(1)}+\mathbf{N}_1\mathbf{t}_g^{(2)},$$

with $\mathbf{t}_g^{(1)}\in I_1$ and $\mathbf{t}_g^{(2)}\in I_2$ determined as above. Suppose further that $\mathbf{N}$, $\mathbf{N}_1$ and $\mathbf{N}_2$ commute with $\mathbf{R}_g$ for all $g\in G$, *i.e.* (by Schur's lemma, Section 1.3.4.2.2.4) that these matrices are integer multiples of the identity in each G-invariant subspace. The action of g on $\mathbf{m}=\mathbf{N}\mathbf{x} \mod \mathbf{N}\mathbb{Z}^3$ leads to

$$\begin{aligned} S_g(\mathbf{m}) &= \mathbf{N}[\mathbf{R}_g(\mathbf{N}^{-1}\mathbf{m})+\mathbf{N}\mathbf{t}_g] && \mod \mathbf{N}\mathbb{Z}^3\\ &= \mathbf{N}\mathbf{R}_g\mathbf{N}^{-1}(\mathbf{m}_1+\mathbf{N}_1\mathbf{m}_2)+\mathbf{t}_g^{(1)}+\mathbf{N}_1\mathbf{t}_g^{(2)} && \mod \mathbf{N}\mathbb{Z}^3\\ &= \mathbf{R}_g\mathbf{m}_1+\mathbf{t}_g^{(1)}+\mathbf{N}_1(\mathbf{R}_g\mathbf{m}_2+\mathbf{t}_g^{(2)}) && \mod \mathbf{N}\mathbb{Z}^3, \end{aligned}$$

which we may decompose as

$$S_g(\mathbf{m})=[S_g(\mathbf{m})]_1+\mathbf{N}_1[S_g(\mathbf{m})]_2$$

with

$$[S_g(\mathbf{m})]_1\equiv S_g(\mathbf{m}) \mod \mathbf{N}_1\mathbb{Z}^3$$

and

$$[S_g(\mathbf{m})]_2\equiv \mathbf{N}_1^{-1}\{S_g(\mathbf{m})-[S_g(\mathbf{m})]_1\} \mod \mathbf{N}_2\mathbb{Z}^3.$$

Introducing the notation

$$\begin{aligned} S_g^{(1)}(\mathbf{m}_1) &= \mathbf{R}_g\mathbf{m}_1+\mathbf{t}_g^{(1)} \mod \mathbf{N}_1\mathbb{Z}^3,\\ S_g^{(2)}(\mathbf{m}_2) &= \mathbf{R}_g\mathbf{m}_2+\mathbf{t}_g^{(2)} \mod \mathbf{N}_2\mathbb{Z}^3, \end{aligned}$$

the two components of $S_g(\mathbf{m})$ may be written

$$\begin{aligned} [S_g(\mathbf{m})]_1 &= S_g^{(1)}(\mathbf{m}_1),\\ [S_g(\mathbf{m})]_2 &= S_g^{(2)}(\mathbf{m}_2)+\boldsymbol{\mu}_2(g,\mathbf{m}_1) \mod \mathbf{N}_2\mathbb{Z}^3, \end{aligned}$$

with

$$\boldsymbol{\mu}_2(g,\mathbf{m}_1)=\mathbf{N}_1^{-1}\{(\mathbf{R}_g\mathbf{m}_1+\mathbf{t}_g^{(1)})-[S_g(\mathbf{m}_1)]_1\} \mod \mathbf{N}_2\mathbb{Z}^3.$$

The term $\boldsymbol{\mu}_2$ is the geometric equivalent of a *carry* or *borrow*: it arises because $\mathbf{R}_g\mathbf{m}_1+\mathbf{t}_g^{(1)}$, calculated as a vector in $\mathbb{Z}^3/\mathbf{N}\mathbb{Z}^3$, may be outside the unit cell $\mathbf{N}_1[0,1]^3$, and may need to be brought back into it by a 'large' translation with a non-zero component in the $\mathbf{m}_2$ space; equivalently, the action of g may need to be applied around different permissible origins for different values of $\mathbf{m}_1$, so as to map the unit cell into itself without any recourse to lattice translations. [Readers familiar with the cohomology of groups (see *e.g.* Hall, 1959; MacLane, 1963) will recognize $\boldsymbol{\mu}_2$ as the cocycle of the extension of $\mathbb{Z}G$-modules described by the exact sequence $0\rightarrow I_2\rightarrow I\rightarrow I_1\rightarrow 0$.]

Thus G acts on I in a rather complicated fashion: although $g \longmapsto S_g^{(1)}$ does define a left action in I_1 alone, no action can be defined in I_2 alone because $\boldsymbol{\mu}_2$ depends on $\mathbf{m}_1$. However, because S_g, $S_g^{(1)}$ and $S_g^{(2)}$ *are* left actions, it follows that $\boldsymbol{\mu}_2$ satisfies the identity

$$\boldsymbol{\mu}_2(gg', \mathbf{m}_1) = S_g^{(2)}[\boldsymbol{\mu}_2(g', \mathbf{m}_1)] + \boldsymbol{\mu}_2[g, S_g^{(1)}(\mathbf{m}_1)] \qquad \text{mod } \mathbf{N}_2\mathbb{Z}^3$$

for all g, g' in G and all $\mathbf{m}_1$ in I_1. In particular, $\boldsymbol{\mu}_2(\mathrm{e}, \mathbf{m}_1) = \mathbf{0}$ for all $\mathbf{m}_1$, and

$$\boldsymbol{\mu}_2(g^{-1}, \mathbf{m}_1) = -S_{g^{-1}}^{(2)}\{\boldsymbol{\mu}_2[g, S_{g^{-1}}^{(1)}(\mathbf{m}_1)]\} \text{ mod } \mathbf{N}_2\mathbb{Z}^3.$$

This action will now be used to achieve optimal use of symmetry in the multidimensional Cooley–Tukey algorithm of Section 1.3.3.3.2.1. Let us form an array Y according to

$$Y(\mathbf{m}_1, \mathbf{m}_2) = \rho(\mathbf{m}_1 + \mathbf{N}_1\mathbf{m}_2)$$

for *all* $\mathbf{m}_2 \in I_2$ but only for the *unique* $\mathbf{m}_1$ under the action $S_g^{(1)}$ of G in I_1. Except in special cases which will be examined later, these vectors contain essentially an asymmetric unit of electron-density data, up to some redundancies on boundaries. We may then compute the partial transform on $\mathbf{m}_2$:

$$Y^*(\mathbf{m}_1, \mathbf{h}_2) = \frac{1}{|\det \mathbf{N}_2|} \sum_{\mathbf{m}_2 \in I_2} Y(\mathbf{m}_1, \mathbf{m}_2) e[\mathbf{h}_2 \cdot (\mathbf{N}_2^{-1}\mathbf{m}_2)].$$

Using the symmetry of ρ in the form $\rho = S_g^{\#}\rho$ yields by the procedure of Section 1.3.3.3.2 the transposition formula

$$Y^*(S_g^{(1)}(\mathbf{m}_1), \mathbf{h}_2) = e\{\mathbf{h}_2 \cdot [\mathbf{N}_2^{-1}(\mathbf{t}_g^{(2)} + \boldsymbol{\mu}_2(g, \mathbf{m}_1))]\} \times Y^*(\mathbf{m}_1, [\mathbf{R}_g^{(2)}]^T\mathbf{h}_2).$$

By means of this identity we can transpose intermediate results Y^* initially indexed by

$$(\text{unique } \mathbf{m}_1) \times (\text{all } \mathbf{h}_2),$$

so as to have them indexed by

$$(\text{all } \mathbf{m}_1) \times (\text{unique } \mathbf{h}_2).$$

We may then apply twiddle factors to get

$$Z(\mathbf{m}_1, \mathbf{h}_2) = e[\mathbf{h}_2 \cdot (\mathbf{N}^{-1}\mathbf{m}_1)] Y^*(\mathbf{m}_1, \mathbf{h}_2)$$

and carry out the second transform

$$Z^*(\mathbf{h}_1, \mathbf{h}_2) = \frac{1}{|\det \mathbf{N}_1|} \sum_{\mathbf{m}_1 \in I_1} Z(\mathbf{m}_1, \mathbf{h}_2) e[\mathbf{h}_1 \cdot (\mathbf{N}_1^{-1}\mathbf{m}_1)].$$

The final results are indexed by

$$(\text{all } \mathbf{h}_1) \times (\text{unique } \mathbf{h}_2),$$

which yield essentially an asymmetric unit of structure factors after unscrambling by:

$$F(\mathbf{h}_2 + \mathbf{N}_2^T\mathbf{h}_1) = Z^*(\mathbf{h}_1, \mathbf{h}_2).$$

The transposition formula above applies to intermediate results when going backwards from F to ρ, provided these results are considered *after* the twiddle-factor stage. A transposition formula applicable *before* that stage can be obtained by characterizing the action of G on $\mathbf{h}$ (including the effects of periodization by $\mathbf{N}^T\mathbb{Z}^3$) in a manner similar to that used for $\mathbf{m}$.

Let

$$\mathbf{h} = \mathbf{h}_2 + \mathbf{N}_2^T\mathbf{h}_1,$$

with

$$\mathbf{h}_2 = \mathbf{h} \qquad \text{mod } \mathbf{N}_2^T\mathbb{Z}^3,$$
$$\mathbf{h}_1 = (\mathbf{N}_2^{-1})^T(\mathbf{h} - \mathbf{h}_2) \quad \text{mod } \mathbf{N}_1^T\mathbb{Z}^3.$$

We may then write

$$\mathbf{R}_g^T\mathbf{h} = [\mathbf{R}_g^T\mathbf{h}]_2 + \mathbf{N}_2^T[\mathbf{R}_g^T\mathbf{h}]_1,$$

with

$$[\mathbf{R}_g^T\mathbf{h}]_2 = [\mathbf{R}_g^{(2)}]^T\mathbf{h}_2 \qquad \text{mod } \mathbf{N}_2^T\mathbb{Z}^3,$$
$$[\mathbf{R}_g^T\mathbf{h}]_1 = [\mathbf{R}_g^{(1)}]^T\mathbf{h}_1 + \boldsymbol{\eta}_1(g, \mathbf{h}_2) \quad \text{mod } \mathbf{N}_1^T\mathbb{Z}^3.$$

Here $[\mathbf{R}_g^{(2)}]^T$, $[\mathbf{R}_g^{(1)}]^T$ and $\boldsymbol{\eta}_1$ are defined by

$$[\mathbf{R}_g^{(2)}]^T\mathbf{h}_2 = \mathbf{R}_g^T\mathbf{h} \qquad \text{mod } \mathbf{N}_2^T\mathbb{Z}^3,$$
$$[\mathbf{R}_g^{(1)}]^T\mathbf{h}_1 = \mathbf{R}_g^T\mathbf{h} \qquad \text{mod } \mathbf{N}_1^T\mathbb{Z}^3$$

and

$$\boldsymbol{\eta}_1(g, \mathbf{h}_2) = (\mathbf{N}_2^{-1})^T(\mathbf{R}_g^T\mathbf{h}_2 - [\mathbf{R}_g^{(2)}]^T\mathbf{h}_2) \text{ mod } \mathbf{N}_1^T\mathbb{Z}^3.$$

Let us then form an array Z^* according to

$$Z^*(\mathbf{h}_1', \mathbf{h}_2') = F(\mathbf{h}_2' + \mathbf{N}_2^T\mathbf{h}_1')$$

for *all* $\mathbf{h}_1'$ but only for the *unique* $\mathbf{h}_2'$ under the action of G in $\mathbb{Z}^3/\mathbf{N}_2^T\mathbb{Z}^3$, and transform on $\mathbf{h}_1'$ to obtain

$$Z(\mathbf{m}_1, \mathbf{h}_2) = \sum_{\mathbf{h}_1' \in \mathbb{Z}^3/\mathbf{N}_1^T\mathbb{Z}^3} Z^*(\mathbf{h}_1', \mathbf{h}_2') e[-\mathbf{h}_1' \cdot (\mathbf{N}_1^{-1}\mathbf{m}_1)].$$

Putting $\mathbf{h}' = \mathbf{R}_g^T\mathbf{h}$ and using the symmetry of F in the form

$$F(\mathbf{h}') = F(\mathbf{h}) \exp(-2\pi i \mathbf{h} \cdot \mathbf{t}_g),$$

where

$$\mathbf{h} \cdot \mathbf{t}_g = (\mathbf{h}_2^T + \mathbf{h}_1^T\mathbf{N}_2)(\mathbf{N}_2^{-1}\mathbf{N}_1^{-1})(\mathbf{t}_g^{(1)} + \mathbf{N}_1\mathbf{t}_g^{(2)})$$
$$\equiv \mathbf{h}_2 \cdot \mathbf{t}_g + \mathbf{h}_2 \cdot (\mathbf{N}_1^{-1}\mathbf{t}_g^{(1)}) \text{ mod } 1$$

yields by a straightforward rearrangement

$$Z(\mathbf{m}_1, [\mathbf{R}_g^{(2)}]^T\mathbf{h}_2) = e[-\{\mathbf{h}_2 \cdot \mathbf{t}_g + \boldsymbol{\eta}_1(g, \mathbf{h}_2) \cdot (\mathbf{N}_1^{-1}\mathbf{m}_1)\}] \times Z\{S_g^{(1)}(\mathbf{m}_1), \mathbf{h}_2\}.$$

This formula allows the transposition of intermediate results Z from an indexing by

$$(\text{all } \mathbf{m}_1) \times (\text{unique } \mathbf{h}_2)$$

to an indexing by

$$(\text{unique } \mathbf{m}_1) \times (\text{all } \mathbf{h}_2).$$

We may then apply the twiddle factors to obtain

$$Y^*(\mathbf{m}_1, \mathbf{h}_2) = e[-\mathbf{h}_2 \cdot (\mathbf{N}^{-1}\mathbf{m}_1)] Z(\mathbf{m}_1, \mathbf{h}_2)$$

and carry out the second transform on $\mathbf{h}_2$

$$Y(\mathbf{m}_1, \mathbf{m}_2) = \sum_{\mathbf{h}_2 \in \mathbb{Z}^3/\mathbf{N}_2^T\mathbb{Z}^3} Y^*(\mathbf{m}_1, \mathbf{h}_2) e[-\mathbf{h}_2 \cdot (\mathbf{N}_2^{-1}\mathbf{m}_2)].$$

The results, indexed by

$$(\text{unique } \mathbf{m}_1) \times (\text{all } \mathbf{m}_2)$$

yield essentially an asymmetric unit of electron densities by the rearrangement

$$\rho(\mathbf{m}_1 + \mathbf{N}_1\mathbf{m}_2) = Y(\mathbf{m}_1, \mathbf{m}_2).$$

The equivalence of the two transposition formulae up to the intervening twiddle factors is readily established, using the relation

$$\mathbf{h}_2 \cdot [\mathbf{N}_2^{-1}\boldsymbol{\mu}_2(g,\mathbf{m}_1)] = \boldsymbol{\eta}_1(g,\mathbf{h}_2)\cdot(\mathbf{N}_1^{-1}\mathbf{m}_1) \bmod 1$$

which is itself a straightforward consequence of the identity

$$\mathbf{h}\cdot[\mathbf{N}^{-1}S_g(\mathbf{m})] = \mathbf{h}\cdot\mathbf{t}_g + (\mathbf{R}_g^T\mathbf{h})\cdot(\mathbf{N}^{-1}\mathbf{m}).$$

To complete the characterization of the effect of symmetry on the Cooley–Tukey factorization, and of the economy of computation it allows, it remains to consider the possibility that some values of $\mathbf{m}_1$ may be invariant under some transformations $g \in G$ under the action $\mathbf{m}_1 \longmapsto S_g^{(1)}(\mathbf{m}_1)$.

Suppose that $\mathbf{m}_1$ has a non-trivial isotropy subgroup $G_{\mathbf{m}_1}$, and let $g \in G_{\mathbf{m}_1}$. Then each subarray $Y_{\mathbf{m}_1}$ defined by

$$Y_{\mathbf{m}_1}(\mathbf{m}_2) = Y(\mathbf{m}_1,\mathbf{m}_2) = \rho(\mathbf{m}_1 + \mathbf{N}_1\mathbf{m}_2)$$

satisfies the identity

$$\begin{aligned} Y_{\mathbf{m}_1}(\mathbf{m}_2) &= Y_{S_g^{(1)}(\mathbf{m}_1)}[S_g^{(2)}(\mathbf{m}_2) + \boldsymbol{\mu}_2(g,\mathbf{m}_1)] \\ &= Y_{\mathbf{m}_1}[S_g^{(2)}(\mathbf{m}_2) + \boldsymbol{\mu}_2(g,\mathbf{m}_1)] \end{aligned}$$

so that the data for the transform on $\mathbf{m}_2$ have residual symmetry properties. In this case the identity satisfied by $\boldsymbol{\mu}_2$ simplifies to

$$\boldsymbol{\mu}_2(gg',\mathbf{m}_1) = S_g^{(2)}[\boldsymbol{\mu}_2(g',\mathbf{m}_1)] + \boldsymbol{\mu}_2(g,\mathbf{m}_1) \bmod \mathbf{N}_2\mathbb{Z}^3,$$

which shows that the mapping $g \longmapsto \boldsymbol{\mu}_2(g,\mathbf{m}_1)$ satisfies the Frobenius congruences (Section 1.3.4.2.2.3). Thus the internal symmetry of subarray $Y_{\mathbf{m}_1}$ with respect to the action of G on $\mathbf{m}_2$ is given by $G_{\mathbf{m}_1}$ acting on $\mathbb{Z}^3/\mathbf{N}_2\mathbb{Z}^3$ *via*

$$\mathbf{m}_2 \longmapsto S_g^{(2)}(\mathbf{m}_2) + \boldsymbol{\mu}_2(g,\mathbf{m}_1) \bmod \mathbf{N}_2\mathbb{Z}^3.$$

The transform on $\mathbf{m}_2$ needs only be performed for one out of $[G : G_{\mathbf{m}_1}]$ distinct arrays $Y_{\mathbf{m}_1}$ (results for the others being obtainable by the transposition formula), and this transforms is $G_{\mathbf{m}_1}$-symmetric. In other words, the following cases occur:

(i)	$G_{\mathbf{m}_1} = \{e\}$	maximum saving in computation (by $\lvert G\rvert$); $\mathbf{m}_2$-transform has no symmetry.
(ii)	$G_{\mathbf{m}_1} = G' < G$	saving in computation by a factor of $[G : G']$; $\mathbf{m}_2$-transform is G'-symmetric.
(iii)	$G_{\mathbf{m}_1} = G$	no saving in computation; $\mathbf{m}_2$-transform is G-symmetric.

The symmetry properties of the $\mathbf{m}_2$-transform may themselves be exploited in a similar way if $\mathbf{N}_2$ can be factored as a product of smaller decimation matrices; otherwise, an appropriate symmetrized DFT routine may be provided, using for instance the idea of 'multiplexing/demultiplexing' (Section 1.3.4.3.5). We thus have a recursive *descent procedure*, in which the deeper stages of the recursion deal with transforms on *fewer points*, or of *lower symmetry* (usually both).

The same analysis applies to the $\mathbf{h}_1$-transforms on the subarrays $Z^*_{\mathbf{h}_2}$, and leads to a similar descent procedure.

In conclusion, crystallographic symmetry can be fully exploited to reduce the amount of computation to the minimum required to obtain the unique results from the unique data. No such analysis was so far available in cases where the asymmetric units in real and reciprocal space are not parallelepipeds. An example of this procedure will be given in Section 1.3.4.3.6.5.

1.3.4.3.4.2. *Multidimensional Good factorization*

This procedure was described in Section 1.3.3.3.2.2. The main difference with the Cooley–Tukey factorization is that if $\mathbf{N} = \mathbf{N}_1\mathbf{N}_2\ldots\mathbf{N}_{d-1}\mathbf{N}_d$, where the different factors are pairwise coprime, then the Chinese remainder theorem reindexing makes $\mathbb{Z}^3/\mathbf{N}\mathbb{Z}^3$ isomorphic to a direct sum.

$$\mathbb{Z}^3/\mathbf{N}\mathbb{Z}^3 \cong (\mathbb{Z}^3/\mathbf{N}_1\mathbb{Z}^3)\oplus\ldots\oplus(\mathbb{Z}^3/\mathbf{N}_d\mathbb{Z}^3),$$

where each p-primary piece is endowed with an induced $\mathbb{Z}G$-module structure by letting G operate in the usual way but with the corresponding modular arithmetic. The situation is thus more favourable than with the Cooley–Tukey method, since there is no interference between the factors (no 'carry'). In the terminology of Section 1.3.4.2.2.2, G acts *diagonally* on this direct sum, and results of a partial transform may be transposed by orbit exchange as in Section 1.3.4.3.4.1 but without the extra terms $\boldsymbol{\mu}$ or $\boldsymbol{\eta}$. The analysis of the symmetry properties of partial transforms also carries over, again without the extra terms. Further simplification occurs for all p-primary pieces with p other than 2 or 3, since all non-primitive translations (including those associated to lattice centring) disappear modulo p.

Thus the cost of the CRT reindexing is compensated by the computational savings due to the absence of twiddle factors and of other phase shifts associated with non-primitive translations and with geometric 'carries'.

Within each p-primary piece, however, higher powers of p may need to be split up by a Cooley–Tukey factorization, or carried out directly by a suitably adapted Winograd algorithm.

1.3.4.3.4.3. *Crystallographic extension of the Rader/Winograd factorization*

As was the case in the absence of symmetry, the two previous classes of algorithms can only factor the global transform into partial transforms on prime numbers of points, but cannot break the latter down any further. Rader's idea of using the action of the group of units $U(p)$ to obtain further factorization of a p-primary transform has been used in 'scalar' form by Auslander & Shenefelt (1987), Shenefelt (1988), and Auslander *et al.* (1988). It will be shown here that it can be adapted to the crystallographic case so as to take advantage also of the possible existence of n-fold cyclic symmetry elements ($n = 3, 4, 6$) in a two-dimensional transform (Bricogne & Tolimieri, 1990). This adaptation entails the use of certain rings of *algebraic* integers rather than ordinary integers, whose connection with the handling of cyclic symmetry will now be examined.

Let G be the group associated with a threefold axis of symmetry: $G = \{e, g, g^2\}$ with $g^3 = e$. In a standard trigonal basis, G has matrix representation

$$\mathbf{R}_e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{I}, \quad \mathbf{R}_g = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \mathbf{R}_{g^2} = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$$

in real space,

$$\mathbf{R}^*_e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{I}, \quad \mathbf{R}^*_g = \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{R}^*_{g^2} = \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}$$

in reciprocal space. Note that

$$\mathbf{R}^*_{g^2} = [\mathbf{R}_{g^2}^{-1}]^T = \mathbf{R}_g^T,$$

and that

$$\mathbf{R}_g^T = \mathbf{J}^{-1}\mathbf{R}_g\mathbf{J}, \quad \text{where } \mathbf{J} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

so that $\mathbf{R}_g$ and $\mathbf{R}_g^T$ are conjugate in the group of 2×2 unimodular

references