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