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The crystallographic fast Fourier transform. III. Centred lattices

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Algorithms for evaluation of the crystallographic FFT for centred lattices are presented. These algorithms can be applied to 80 space groups containing centring operators. For 44 of them, combining these algorithms with those described by Rowicka, Kudlicki & Otwinowski [*Acta Cryst* A**59**, 172–182] yields the maximal symmetry reduction. For other groups, new algorithms, to be presented in our forthcoming paper [Rowicka, Kudlicki & Otwinowski (2003), in preparation], are needed. The requirements on the grid size and how they interact with the choice of algorithms are also discussed in detail.

1. Introduction

This is the third in the series of articles describing our algorithms for evaluation of the crystallographic fast Fourier transform (FFT). Recently, we have presented explicit schemes for one-step symmetry reduction for 67 space groups in papers I and II (Rowicka *et al.*, 2002, 2003*a*). As many as 80 of the remaining space groups contain centring translations. We devote this paper to reducing symmetry induced by these centrings. We will show how to achieve maximal symmetry reduction for 44 groups. To this end, we will combine the symmetry-reduction formula presented in paper II with the here presented algorithms that take care of centring. To achieve maximal symmetry reduction for the remaining 36 groups containing centring operators, the algorithm described has to be combined with a new scheme dealing with data points in special positions. Such a scheme will be presented in paper IV (Rowicka *et al.*, 2003*b*).

The article is organized as follows. In §2, we introduce mathematical notions and notation we will use later on. In §3, we propose algorithms for centred lattices. In §4, we offer remarks on how different choices of algorithms restrict grid sizes. Next, in §5, we show how to combine the symmetry-reduction formula with the treatment of centred lattices. In §6, requirements, limitations and future development and application of our algorithms are discussed. In Appendices *A* and *B*, we provide detailed description of the algorithm for specific crystallographic groups.

2. Mathematical notions and notation

As in paper II, we follow the modern approach of Bricogne (1993) and hence use a similar notation. Let $\mathbb{Z}$ denote the set of all integers and $\mathbb{Z}^3$ denote the Cartesian product $\mathbb{Z}\times\mathbb{Z}\times\mathbb{Z}$. Matrices and vectors will be written in bold type. The standard basis vectors of $\mathbb{Z}^3$ will be denoted by $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$. Our goal is to compute discrete Fourier transforms of a periodic function f defined on $\mathbb{Z}^3$. Such a function will have the periodicity of the underlying crystal structure, described by a 3×3 matrix with integer entries, $\mathbf{A}$. From now on, we will require that $\mathbf{A}$ be invertible (that is, that its determinant is not equal to zero: $\det\mathbf{A}\neq 0$). The periodicity condition reads

$$f(\mathbf{x}+\mathbf{t})=f(\mathbf{x}),$$

where $\mathbf{x}\in\mathbb{Z}^3$ and

$$\mathbf{t}\in\mathbf{A}\mathbb{Z}^3=\{\mathbf{x}\in\mathbb{Z}^3:\ \text{there exists a }\ \mathbf{y}\in\mathbb{Z}^3\ \text{such that}\ \mathbf{x}=\mathbf{A}\mathbf{y}\}.$$

As in paper II, we will use the following *equivalence relation*:

$$\mathbf{y}\mathcal{R}_{\mathbf{A}}\mathbf{x}\Leftrightarrow\mathbf{y}-\mathbf{x}\in\mathbf{A}\mathbb{Z}^3.$$

This means that $\mathbf{x}$ and $\mathbf{y}$ are in the relation $\mathcal{R}_{\mathbf{A}}$ if and only if they have the same crystallographic coordinates. The equivalence class of $\mathbf{x}$ (with respect to the relation $\mathcal{R}_{\mathbf{A}}$) will be

$$[\mathbf{x}]_{\mathbf{A}}=\{\mathbf{y}\in\mathbb{Z}^3\ :\ \mathbf{y}-\mathbf{x}\in\mathbf{A}\mathbb{Z}^3\}.$$

Another useful notion is that of a *quotient space* (see also Rowicka *et al.*, 2003*a*; Bricogne, 1993). In this article, we deal with the quotient space of $\mathbb{Z}^3$ by $\mathbf{A}\mathbb{Z}^3$:

$$\mathbb{Z}^3/\mathbf{A}\mathbb{Z}^3=\{[\mathbf{x}]_{\mathbf{A}}:\ \mathbf{x}\in\mathbb{Z}^3\}.$$

The notion of a quotient space allows us to describe periodicity conditions in a very convenient way. Instead of viewing f as a periodic function, it can be equivalently considered as defined on the set of the equivalence classes, $\mathbb{Z}^3/\mathbf{A}\mathbb{Z}^3$. Let us introduce the notation

$$\Gamma=\mathbb{Z}^3/\mathbf{A}\mathbb{Z}^3 \tag{1}$$

and

$$\Gamma^*=\mathbb{Z}^3/\mathbf{A}^T\mathbb{Z}^3,$$

where $\mathbf{A}^T$ denotes the transposition of matrix $\mathbf{A}$. The space Γ^* is a space dual to Γ. Its elements are covectors, *i.e.* objects dual to vectors. Covectors will also be printed in bold type and they will be, when there is no risk of confusion, also referred to as

vectors. The scalar product of a covector $\mathbf{h} \in \Gamma^*$ and a vector $\mathbf{x} \in \Gamma$, expressed in standard bases, reads

$$\mathbf{h} \cdot \mathbf{x} = (h\mathbf{e}_1^* + k\mathbf{e}_2^* + l\mathbf{e}_3^*) \cdot (x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3) = hx + ky + lz,$$

where $h, k, l, x, y, z \in \mathbb{Z}$. We shall use a shorthand notation $e_{\mathbf{A}}(\mathbf{h}, \mathbf{x})$ for a coefficient (also called 'twiddle factor') that will occur frequently throughout this paper:

$$e_{\mathbf{A}}(\mathbf{h}, \mathbf{x}) = \exp(-2\pi i \mathbf{h} \cdot \mathbf{A}^{-1}\mathbf{x}).$$

This symbol has the following properties:

$$e_{\mathbf{A}}(\mathbf{g} + \mathbf{h}, \mathbf{x}) = e_{\mathbf{A}}(\mathbf{g}, \mathbf{x}) e_{\mathbf{A}}(\mathbf{h}, \mathbf{x})$$
$$e_{\mathbf{A}}(\mathbf{h}, \mathbf{x} + \mathbf{y}) = e_{\mathbf{A}}(\mathbf{h}, \mathbf{x}) e_{\mathbf{A}}(\mathbf{h}, \mathbf{y})$$

for any $\mathbf{g}, \mathbf{h} \in \Gamma^*$ and $\mathbf{x}, \mathbf{y} \in \Gamma$. Let f be a complex-valued function on Γ, where Γ is given by (1). The Fourier transform of function f will be denoted by F and for any $\mathbf{h} \in \Gamma^*$ defined by

$$F(\mathbf{h}) = \sum_{\mathbf{x} \in \Gamma} f(\mathbf{x}) e_{\mathbf{A}}(\mathbf{h}, \mathbf{x}). \tag{2}$$

For simplicity, in the above formula, we have omitted the normalization constant $1/|\det \mathbf{A}|$.

2.1. Crystallographic group action

Let G denote the quotient (or factor) crystallographic space group (Bricogne, 1993; Rowicka *et al.*, 2003*a*). The elements of G are the symmetry operators as listed in *International Tables for Crystallography* (ITC) (Hahn, 1995). The group operation in G is the ordinary composition of symmetry operators.

We represent the action of an element $g \in G$ in the real space as follows:

$$S_g(\mathbf{x}) = \mathbf{R}_g \mathbf{x} + \mathbf{t}_g, \tag{3}$$

where $\mathbf{x} \in \Gamma$. We will call $\mathbf{R}_g$ the rotational part of the symmetry operator related to g. Since $\det \mathbf{R}_g = \pm 1$, it follows that $\mathbf{R}_g$ can be either a proper ($\det \mathbf{R}_g = 1$) or an improper ($\det \mathbf{R}_g = -1$) rotation. We will call $\mathbf{t}_g$ a translational part of the symmetry operator. We stress again that, since $\mathbf{x} \in \Gamma = \mathbb{Z}^3/\mathbf{A}\mathbb{Z}^3$, the symbol $\mathbf{x}$ in the formula above is in fact the equivalence class $[\mathbf{x}]_{\mathbf{A}}$. The action (3) defines an action $S^{\#}$ on a function f on space Γ by

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

This action $S^{\#}$ on the functions in the real space extends to the action S^* on their Fourier transforms in the reciprocal space:

$$S_g^* F(\mathbf{h}) = e_{\mathbf{A}}(\mathbf{h}, \mathbf{t}_g) F(\mathbf{R}_g^T \mathbf{h}). \tag{4}$$

3. Algorithms

In paper II, the symmetry-reduction formula combining the multidimensional Cooley–Tukey factorization with crystallographic symmetry was derived, and the conditions of its use were discussed. It was shown that for some groups this formula allows maximal symmetry reduction to be achieved in one step.

However, after performing this symmetry reduction what may remain in some space groups is a non-primitive translational symmetry (centring). These are the cases this article deals with. No asymmetric unit in such cases can be described by a decomposition matrix [such as $\mathbf{A}_0$ in formula (10) of paper II], as opposed to the space groups we considered so far. As a result, the centring operators cannot be treated by the Cooley–Tukey type of decomposition.

Therefore, we propose a set of algorithms to treat centring-induced symmetry. This time, we choose an asymmetric unit that will be a contiguous set. It will be similar to FFT-asymmetric units in the reciprocal space in paper II. One can also associate a matrix with it, but the relationship between the grid and its matrix will be different from that in paper II. One can expect that the size of the asymmetric unit will be $1/|G|$, where $|G|$ is the number of elements in the subgroup generated by the centring symmetry operators. However, as will become clear soon, it is more convenient to choose as an asymmetric unit only half, one-quarter or even one-ninth of these points, but consider two, four or nine, respectively,

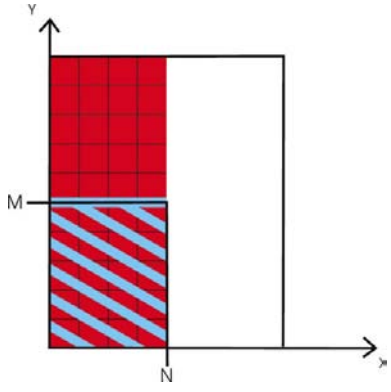

Figure 1
C-face centring, real space. Section at $z = 0$ is shown. The asymmetric unit is coloured red. The dashed area is the domain of definition of functions f_1 and f_2.

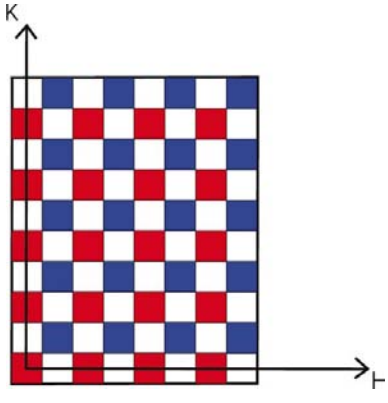

Figure 2
C-face centring, reciprocal space. Section at $l = 0$. Centres of colored squares form the FFT-asymmetric unit, red squares symbolize $F_1(\mathbf{h}_0)$ and blue ones $F_2(\mathbf{h}_0)$. The Fourier transform equals zero at the centres of white squares.

independent functions on these points. Thus the same amount of information is encoded, but in a more convenient way. We will use similar methods to deal with all types of centrings. We will treat the centring-induced symmetry reduction as an independent step. It means that, for a given crystallographic group, we take a subgroup generated by centring operators as our starting symmetry group. We will also introduce new matrices $\mathbf{A}$, describing conditions imposed on the computational grid solely by centring operators. The symbols $\mathbf{A}_C$, $\mathbf{A}_A$, $\mathbf{A}_F$, $\mathbf{A}_I$ and $\mathbf{A}_R$ will denote matrices describing computational grids for C-face centring, A-face centring, all-face centring, body centring and rhombohedral centring, respectively:

$$\mathbf{A}_C = \begin{bmatrix} 2N & 0 & 0 \\ 0 & 2M & 0 \\ 0 & 0 & Q \end{bmatrix}, \quad \mathbf{A}_A = \begin{bmatrix} N & 0 & 0 \\ 0 & 2M & 0 \\ 0 & 0 & 2Q \end{bmatrix},$$

$$\mathbf{A}_F = \mathbf{A}_I = \begin{bmatrix} 2N & 0 & 0 \\ 0 & 2M & 0 \\ 0 & 0 & 2Q \end{bmatrix}, \quad \mathbf{A}_R = \begin{bmatrix} 3N & 0 & 0 \\ 0 & 3M & 0 \\ 0 & 0 & 3Q \end{bmatrix},$$

where N, M and Q are positive integers. In each of the subsequent subsections, dealing with a specific centring, we will omit indices in matrices $\mathbf{A}$ indicating the centring type.

Let T_x, T_y and T_z denote non-primitive translation operators

$$(T_x f)(\mathbf{x}) = f(\mathbf{x} + N\mathbf{e}_1)$$
$$(T_y f)(\mathbf{x}) = f(\mathbf{x} + M\mathbf{e}_2)$$
$$(T_z f)(\mathbf{x}) = f(\mathbf{x} + Q\mathbf{e}_3).$$

Let I denote the identity operator. Then, for all centring types except for rhombohedral centring,

$$T_x^2 = \mathrm{I} \quad \text{and} \quad T_y^2 = \mathrm{I} \quad \text{and} \quad T_z^2 = \mathrm{I}.$$

For the rhombohedral centring,

$$T_x^3 = \mathrm{I} \quad \text{and} \quad T_y^3 = \mathrm{I} \quad \text{and} \quad T_z^3 = \mathrm{I}.$$

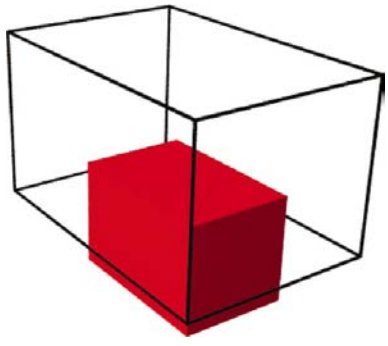

Figure 3
All-face centring, real space. The set $\tilde{\Gamma}_0$, the domain of definition of functions f_1 and f_2 is coloured red. Its volume is one-eighth of the unit cell, it corresponds to half of the asymmetric unit.

3.1. *C*-face centred lattices

Here $\mathbf{A} = \mathbf{A}_C$. This type of centring occurs whenever the crystallographic group contains the operator $x + \frac{1}{2}, y + \frac{1}{2}, z$. In this case, the asymmetric unit may be chosen to consist of all grid points that have coordinates in the following range: $x = 0, \ldots, N-1$, $y = 0, \ldots, 2M-1$ and $z = 0, \ldots, Q-1$. The asymmetric unit described above is presented in Fig. 1.

To have a more concise notation for this kind of subset, let us introduce matrices

$$\tilde{\mathbf{A}}_0 = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \tilde{\mathbf{A}}_1 = \begin{bmatrix} N & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & Q \end{bmatrix},$$

such that

$$\mathbf{A} = \tilde{\mathbf{A}}_1 \tilde{\mathbf{A}}_0.$$

Let $\tilde{\Gamma}_0$ be

$$\tilde{\Gamma}_0 = \mathbb{Z}^3 / \tilde{\mathbf{A}}_1 \mathbb{Z}^3.$$

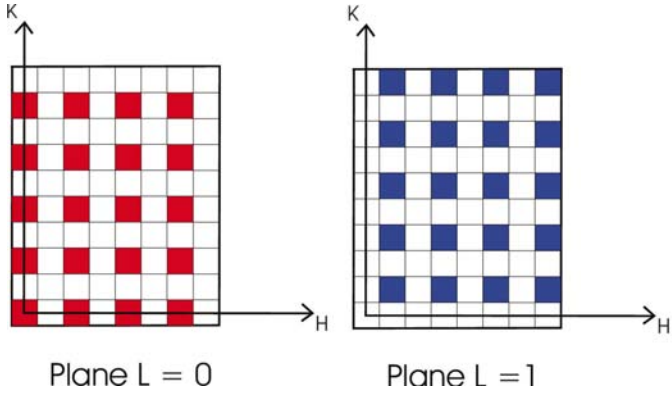

Figure 4
FFT-asymmetric unit in the reciprocal space for all-face centring. The Fourier transform behaves differently in planes with l even (left panel) and l odd (right panel). The Fourier transform equals zero in the centres of blank squares. Centres of the coloured squares form the FFT-asymmetric unit in the reciprocal space. Red denotes $F_1(\mathbf{h}_0)$ and blue denotes $F_2(\mathbf{h}_0)$.

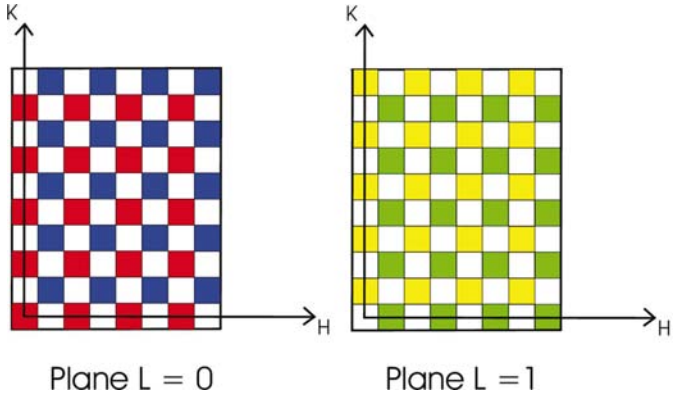

Figure 5
FFT-asymmetric unit in the reciprocal space for body centring. The Fourier transform equals zero in different places depending on the parity of coordinate l. $F_1(\mathbf{h}_0)$ is denoted red, $F_2(\mathbf{h}_0)$ is denoted blue, $F_3(\mathbf{h}_0)$ is denoted green and $F_4(\mathbf{h}_0)$ is denoted yellow.

The tilde above the matrix symbol Γ_0 indicates that Γ_0 from paper II is not the same as $\tilde{\Gamma}_0$ here, and that the above relationship between $\tilde{\mathbf{A}}_1$ and $\tilde{\Gamma}_0$ is different from that between $\mathbf{A}_1$ and Γ_0 described in paper II.

Let us compute the Fourier transform

$$\begin{aligned}F(\mathbf{h}) = \sum_{\mathbf{x}\in\Gamma} f(\mathbf{x})e_{\mathbf{A}}(\mathbf{h},\mathbf{x}) = \sum_{\mathbf{x}\in\tilde{\Gamma}_0} \{&f(\mathbf{x})e_{\mathbf{A}}(\mathbf{h},\mathbf{x})\\ &+ (T_xT_yf)(\mathbf{x})e_{\mathbf{A}}(\mathbf{h},(\mathbf{x}+N\mathbf{e}_1+M\mathbf{e}_2))\\ &+ (T_yf)(\mathbf{x})e_{\mathbf{A}}(\mathbf{h},(\mathbf{x}+M\mathbf{e}_2)) + (T_xf)(\mathbf{x})e_{\mathbf{A}}(\mathbf{h},(\mathbf{x}+N\mathbf{e}_1))\}.\end{aligned}$$

Note that

$$\begin{aligned}e_{\mathbf{A}}(\mathbf{h},(\mathbf{x}+M\mathbf{e}_2)) &= \exp(-k\pi i)e_{\mathbf{A}}(\mathbf{h},\mathbf{x})\\ e_{\mathbf{A}}(\mathbf{h},(\mathbf{x}+N\mathbf{e}_1+M\mathbf{e}_2)) &= \exp[-(h+k)\pi i]e_{\mathbf{A}}(\mathbf{h},\mathbf{x})\\ e_{\mathbf{A}}(\mathbf{h},(\mathbf{x}+N\mathbf{e}_1)) &= \exp(-h\pi i)e_{\mathbf{A}}(\mathbf{h},\mathbf{x}).\end{aligned}$$

Moreover, by symmetry,

$$f(\mathbf{x}) = (T_xT_yf)(\mathbf{x}).$$

Thus,

$$\begin{aligned}F(\mathbf{h}) = &\sum_{\mathbf{x}\in\tilde{\Gamma}_0} \{1+\exp[-\pi i(h+k)]\}e_{\mathbf{A}}(\mathbf{h},\mathbf{x})f(\mathbf{x})\\ &+ \sum_{\mathbf{x}\in\tilde{\Gamma}_0} \exp(-\pi ik)\{1+\exp[-\pi i(h+k)]\}e_{\mathbf{A}}(\mathbf{h},\mathbf{x})(T_yf)(\mathbf{x}).\end{aligned} \tag{5}$$

Analogously as in paper II, one can uniquely decompose $\mathbf{h}$ as

$$\mathbf{h} = \tilde{\mathbf{A}}_0\mathbf{h}_0 + \mathbf{h}_1, \tag{6}$$

where $\mathbf{h}_0 \in \mathbb{Z}^3/\tilde{\mathbf{A}}_1\mathbb{Z}^3$ and $\mathbf{h}_1 \in \mathbb{Z}^3/\tilde{\mathbf{A}}_0\mathbb{Z}^3 = \{\mathbf{0}, \mathbf{e}_1^*, \mathbf{e}_2^*, \mathbf{e}_1^*+\mathbf{e}_2^*\}$. Hence, taking into account the formula (5), we obtain

$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_1^*) = 0 \quad \text{and} \quad F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_2^*) = 0.$$

For $\mathbf{x}\in\tilde{\Gamma}_0$, let us define

$$\begin{aligned}f_1(\mathbf{x}) &= 2(\{f(\mathbf{x})+(T_yf)(\mathbf{x})\}) = 2(\{\mathrm{I}+T_y\}f)(\mathbf{x})\\ f_2(\mathbf{x}) &= 2e_{\mathbf{A}}((\mathbf{e}_1^*+\mathbf{e}_2^*),\mathbf{x})\{f(\mathbf{x})-(T_yf)(\mathbf{x})\}\\ &= 2e_{\mathbf{A}}((\mathbf{e}_1^*+\mathbf{e}_2^*),\mathbf{x})(\{\mathrm{I}-T_y\}f)(\mathbf{x}).\end{aligned}$$

With this notation,

$$\begin{aligned}F(\tilde{\mathbf{A}}_0\mathbf{h}_0) &= \sum_{\mathbf{x}\in\tilde{\Gamma}_0} f_1(\mathbf{x})e_{\mathbf{A}}(\tilde{\mathbf{A}}_0\mathbf{h}_0,\mathbf{x}) = F_1(\mathbf{h}_0)\\ F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_1^*+\mathbf{e}_2^*) &= \sum_{\mathbf{x}\in\tilde{\Gamma}_0} f_2(\mathbf{x})e_{\mathbf{A}}(\tilde{\mathbf{A}}_0\mathbf{h}_0,\mathbf{x}) = F_2(\mathbf{h}_0).\end{aligned}$$

This means that, in order to evaluate the Fourier transform of f on the computational grid defined by Γ, it is enough to compute Fourier transforms F_1 and F_2 of functions f_1 and f_2 on the computational grid defined by $\tilde{\Gamma}_0$. The size of this grid is one-quarter of that of the original grid. The FFT-asymmetric unit in the reciprocal space (see paper II for definition) is shown in Fig. 2.

This algorithm is denoted by CCent. in Appendix *A*.

3.2. *A*-face centred lattices

In this subsection, $\mathbf{A} = \mathbf{A}_A$. Now the symmetry operator is $x, y+\frac{1}{2}, z+\frac{1}{2}$, so the entire reasoning remains the same as in the previous case, we only substitute z coordinates for x coordinates. In particular, the functions f_1 and f_2 are given by

$$\begin{aligned}f_1(\mathbf{x}) &= 2(\{\mathrm{I}+T_z\}f)(\mathbf{x})\\ f_2(\mathbf{x}) &= 2e_{\mathbf{A}}((\mathbf{e}_2^*+\mathbf{e}_3^*),\mathbf{x})(\{\mathrm{I}-T_z\}f)(\mathbf{x}).\end{aligned}$$

This algorithm is denoted by ACent. in Appendix *A*.

3.3. All-face centred lattices

Here $\mathbf{A} = \mathbf{A}_F$. Such a centring occurs whenever the symmetry operators $x, y+\frac{1}{2}, z+\frac{1}{2}$ (inducing *C*-face centring) and $x+\frac{1}{2}, y+\frac{1}{2}, z$ (inducing *A*-face centring) appear together. In this case, we choose $\tilde{\mathbf{A}}_0 = 2\mathbf{I}_3$, where $\mathbf{I}_3$ denotes the 3×3 identity matrix. Then, $\tilde{\mathbf{A}}_1 = \mathbf{A}\tilde{\mathbf{A}}_0^{-1}$. As usual, $\tilde{\Gamma}_0 = \mathbb{Z}^3/\tilde{\mathbf{A}}_1\mathbb{Z}^3$ (Fig. 3).

Let us denote

$$\begin{aligned}f_1(\mathbf{x}) &= 4(\{\mathrm{I}+T_z\}f)(\mathbf{x})\\ f_2(\mathbf{x}) &= 4e_{\mathbf{A}}(\mathbf{e}_1^*,\mathbf{x})(\{\mathrm{I}-T_z\}f)(\mathbf{x}).\end{aligned}$$

These functions are defined on $\tilde{\Gamma}_0$, which is depicted in Fig. 3. Then, for $\mathbf{h}_0 \in \mathbb{Z}^3/\tilde{\mathbf{A}}_1\mathbb{Z}^3$, we have

$$\begin{aligned}F(\tilde{\mathbf{A}}_0\mathbf{h}_0) &= F_1(\mathbf{h}_0)\\ F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_1^*+\mathbf{e}_2^*+\mathbf{e}_3^*) &= F_2(\mathbf{h}_0).\end{aligned}$$

This provides a recipe for the Fourier transform in points of the reciprocal space whose coordinates are either all even or all odd. It can be shown that the Fourier transform equals zero in all other points of the FFT unit cell, namely

$$\begin{aligned}F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_1^*) &= 0\\ F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_2^*) &= 0\\ F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_3^*) &= 0\\ F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_1^*+\mathbf{e}_2^*) &= 0\\ F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_1^*+\mathbf{e}_3^*) &= 0\\ F(\tilde{\mathbf{A}}_0\mathbf{h}_0+\mathbf{e}_2^*+\mathbf{e}_3^*) &= 0.\end{aligned}$$

The FFT-asymmetric unit in the reciprocal space is shown in Fig. 4. This algorithm is denoted by FCent. in Appendix *A*.

3.4. Body-centred lattices

Here, $\mathbf{A} = \mathbf{A}_I$. This centring is related to the operator $x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$. In this case, we also choose $\tilde{\mathbf{A}}_0 = 2\mathbf{I}_3$. As usual, $\tilde{\mathbf{A}}_1 = \mathbf{A}\mathbf{A}_0^{-1}$. Let us define the following functions:

$$\begin{aligned}f_1(\mathbf{x}) &= 2(\{\mathrm{I}+T_xf+T_y+T_z\}f)(\mathbf{x})\\ f_2(\mathbf{x}) &= 2e_{\mathbf{A}}((\mathbf{e}_1^*+\mathbf{e}_2^*),\mathbf{x})(\{\mathrm{I}-T_x-T_y+T_z\}f)(\mathbf{x})\\ f_3(\mathbf{x}) &= 2e_{\mathbf{A}}((\mathbf{e}_1^*+\mathbf{e}_3^*),\mathbf{x})(\{\mathrm{I}-T_x+T_y-T_z\}f)(\mathbf{x})\\ f_4(\mathbf{x}) &= 2e_{\mathbf{A}}((\mathbf{e}_2^*+\mathbf{e}_3^*),\mathbf{x})(\{\mathrm{I}+T_x-T_y-T_z\}f)(\mathbf{x}).\end{aligned}$$

Then, for $\mathbf{h}_0 \in \mathbb{Z}^3/\tilde{\mathbf{A}}_1\mathbb{Z}^3$, the Fourier transform F is expressed in terms of the Fourier transforms of functions f_1, f_2, f_3 and f_4 as follows:

$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0) = F_1(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + \mathbf{e}_1^* + \mathbf{e}_2^*) = F_2(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + \mathbf{e}_1^* + \mathbf{e}_3^*) = F_3(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + \mathbf{e}_2^* + \mathbf{e}_3^*) = F_4(\mathbf{h}_0).$$

Moreover, it can be shown that the Fourier transform equals 0 in all other points of the FFT unit cell. The FFT-asymmetric unit in the reciprocal space is shown in Fig. 5. This algorithm is denoted by ICent. in Appendix *A*.

3.5. Rhombohedral centring

This centring is induced by symmetry operators: $x+\frac{2}{3}, y+\frac{1}{3}, z+\frac{1}{3}$ and $x+\frac{1}{3}, y+\frac{2}{3}, z+\frac{2}{3}$ (obverse setting). In such a case,

$$\mathbf{A} = \begin{bmatrix} 3N & 0 & 0 \\ 0 & 3M & 0 \\ 0 & 0 & 3Q \end{bmatrix},$$

where N, M and Q are positive integers. We choose $\tilde{\mathbf{A}}_0$ to be $3\mathbf{I}_3$. In solving this case, we follow the same simple rules as in the previously discussed centrings. The resulting formulae look much more complicated, although the underlying logic is the same. Note that, unlike before, in this subsection T_z denotes a translation along the z axis by $\frac{1}{3}$ of the unit-cell size and T_z^2 by $\frac{2}{3}$. The same holds for T_y and T_y^2. Let us define

$$\tilde{f}_1(\mathbf{x}) = f(\mathbf{x}) + T_z f(\mathbf{x}) + T_z^2 f(\mathbf{x})$$
$$\tilde{f}_2(\mathbf{x}) = f(\mathbf{x}) + \exp(2\pi i/3) T_z f(\mathbf{x}) + \exp(4\pi i/3) T_z^2 f(\mathbf{x})$$
$$\tilde{f}_3(\mathbf{x}) = f(\mathbf{x}) + \exp(4\pi i/3) T_z f(\mathbf{x}) + \exp(2\pi i/3) T_z^2 f(\mathbf{x}).$$

Now, the functions $f_1, \ldots, f_9$, whose Fourier transforms $F_1, \ldots, F_9$ have to be computed, are given by

$$f_1(\mathbf{x}) = (\{\mathrm{I} + T_y + T_y^2\}\tilde{f}_1)(\mathbf{x})$$
$$f_2(\mathbf{x}) = 3e_{\mathbf{A}}((\mathbf{e}_2^* + 2\mathbf{e}_3^*), \mathbf{x})(\{\mathrm{I} + \exp(4\pi i/3) T_y + \exp(2\pi i/3) T_y^2\}\tilde{f}_2)(\mathbf{x})$$
$$f_3(\mathbf{x}) = 3e_{\mathbf{A}}((2\mathbf{e}_2^* + \mathbf{e}_3^*), \mathbf{x})(\{\mathrm{I} + \exp(2\pi i/3) T_y + \exp(4\pi i/3) T_y^2\}\tilde{f}_3)(\mathbf{x})$$
$$f_4(\mathbf{x}) = 3e_{\mathbf{A}}((\mathbf{e}_1^* + \mathbf{e}_3^*), \mathbf{x})(\{\mathrm{I} + T_y + T_y^2\}\tilde{f}_3)(\mathbf{x})$$
$$f_5(\mathbf{x}) = 3e_{\mathbf{A}}((\mathbf{e}_1^* + \mathbf{e}_2^*), \mathbf{x})(\{\mathrm{I} + \exp(4\pi i/3) T_y + \exp(2\pi i/3) T_y^2\}\tilde{f}_1)(\mathbf{x})$$
$$f_6(\mathbf{x}) = 3e_{\mathbf{A}}((\mathbf{e}_1^* + 2\mathbf{e}_2^* + 2\mathbf{e}_3^*), \mathbf{x})(\{\mathrm{I} + \exp(2\pi i/3) T_y + \exp(4\pi i/3) T_y^2\}\tilde{f}_2)(\mathbf{x})$$
$$f_7(\mathbf{x}) = 3e_{\mathbf{A}}((2\mathbf{e}_1^* + 2\mathbf{e}_3^*), \mathbf{x})(\{\mathrm{I} + T_y + T_y^2\}\tilde{f}_2)(\mathbf{x})$$
$$f_8(\mathbf{x}) = 3e_{\mathbf{A}}((2\mathbf{e}_1^* + \mathbf{e}_2^* + \mathbf{e}_3^*), \mathbf{x})(\{\mathrm{I} + \exp(4\pi i/3) T_y + \exp(2\pi i/3) T_y^2\}\tilde{f}_3)(\mathbf{x})$$
$$f_9(\mathbf{x}) = 3e_{\mathbf{A}}((2\mathbf{e}_1^* + 2\mathbf{e}_2^*), \mathbf{x})(\{\mathrm{I} + \exp(2\pi i/3) T_y + \exp(4\pi i/3) T_y^2\}\tilde{f}_1)(\mathbf{x}).$$

Then,

$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0) = F_1(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + \mathbf{e}_2^* + 2\mathbf{e}_3^*) = F_2(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + 2\mathbf{e}_2^* + \mathbf{e}_3^*) = F_3(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + \mathbf{e}_1^* + \mathbf{e}_3^*) = F_4(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + \mathbf{e}_1^* + \mathbf{e}_2^*) = F_5(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + \mathbf{e}_1^* + 2\mathbf{e}_2^* + 2\mathbf{e}_3^*) = F_6(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + 2\mathbf{e}_1^* + 2\mathbf{e}_3^*) = F_7(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + 2\mathbf{e}_1^* + \mathbf{e}_2^* + \mathbf{e}_3^*) = F_8(\mathbf{h}_0)$$
$$F(\tilde{\mathbf{A}}_0\mathbf{h}_0 + 2\mathbf{e}_1^* + 2\mathbf{e}_2^*) = F_9(\mathbf{h}_0).$$

Moreover, it can be shown that the Fourier transform equals 0 in all the other points of the FFT unit cell, that is in points (h, k, l) such that $2h + k + l$ is not divisible by 3.

4. Combining centring with decimation: example of *C*2 group

As we have stated in §3, the crystallographic groups we deal with in this paper have a subgroup whose symmetry can be maximally reduced by using the formalism described in paper II. Let us denote this subgroup by G_{NT} and a subgroup generated by the non-primitive translation operators by G_{CL}. Then, since G_{CL} is a normal subgroup of G, one can consider a quotient group G/G_{CL}. This quotient group coincides with G_{NT}. By definition, it will not contain any purely translational symmetry operators. Consequently, one can apply to it the approach developed in §§3 and 4 of paper II. Let us explain this procedure by the example of the *C*2 space group. The symmetry operators for this group (in the crystallographic coordinates) are

$$e: \quad x, y, z$$
$$\alpha: \quad -x, y, -z$$
$$\beta: \quad x+\tfrac{1}{2}, y+\tfrac{1}{2}, z$$
$$\alpha\beta: \quad -x+\tfrac{1}{2}, y+\tfrac{1}{2}, -z.$$

The fourth operator is denoted by $\alpha\beta$, because it is a composition of the second and the third ones. Then,

$$G = \{e, \alpha, \beta, \alpha\beta\}.$$

The subgroup generated by translations, G_{CL}, is given by

$$G_{\mathrm{CL}} = \{e, \beta\}.$$

Therefore,

$$G_{\mathrm{NT}} = G/G_{\mathrm{CL}} = \{e, \alpha\}.$$

Let us deal first with the symmetry induced by G/G_{CL}, and only then with the *C*-face centring (that is G_{CL}). This procedure is depicted in Appendix *A* by

Name	Vector $-\mathbf{b}$	Matrix $\mathbf{A}$	Algorithm
*C*2	$(0, 0, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2z CCent.

Here, the matrix $\mathbf{A}$ and the vector $\mathbf{b}$ define the change from crystallographic to the grid coordinates. Let $\mathbf{x}^c$ and $\mathbf{x}$ denote

the coordinates of the same point in the crystallographic and grid coordinate systems, respectively. The transformation from the crystallographic to the grid coordinates is then given by

$$\mathbf{x} = \mathbf{A}\mathbf{x}^c + \mathbf{b}. \tag{7}$$

The matrix $\mathbf{A}$ here is the same matrix that described the grid Γ [see equation (1)]. The vector $\mathbf{b}$ corresponds to the shift of the origin of the coordinate system.

The expression $2|x, 2|y, 2|z$ in the third column means that the number of points along x, y and z axes should be even. Consequently,

$$\mathbf{A} = \begin{bmatrix} 2N & 0 & 0 \\ 0 & 2M & 0 \\ 0 & 0 & 2Q \end{bmatrix} \quad \text{and} \quad \mathbf{b} = -\begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix},$$

where N, M and Q are positive integers.

The relationship between the symmetry operator $(\mathbf{R}_g^c, \mathbf{t}_g^c)$ in the crystallographic coordinate system and in the grid coordinate system $(\mathbf{R}_g, \mathbf{t}_g)$ is the following:

$$\mathbf{R}_g = \mathbf{R}_g^c \quad \text{and} \quad \mathbf{t}_g = (\mathbf{I} - \mathbf{R}_g^c)\mathbf{b} + \mathbf{A}\mathbf{t}_g^c.$$

Hence, in our case,

$$\mathbf{R}_\alpha = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \mathbf{t}_\alpha = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}.$$

Moreover, 2z in the column Algorithm means that $\mathbf{A}_0$ is given by

$$\mathbf{A}_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

As a result,

$$\mathbf{A}_1 = \begin{bmatrix} 2N & 0 & 0 \\ 0 & 2M & 0 \\ 0 & 0 & Q \end{bmatrix}.$$

Let us decompose $\mathbf{h}$ according to the formula

$$\mathbf{h} = \mathbf{h}_1 + \mathbf{A}_1\mathbf{h}_0,$$

where

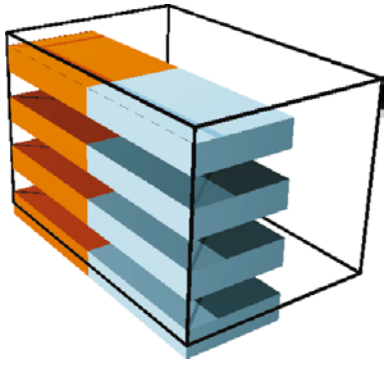

Figure 6
The 2z CCent. decomposition for the $C2$ group. The asymmetric unit is the area coloured orange or blue; the domain of definition of functions f_1 and f_2 is blue.

$$\mathbf{h}_0 \in \mathbb{Z}^3/\mathbf{A}_1\mathbb{Z}^3 = \left\{ \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$$

and

$$\mathbf{h}_1 \in \mathbb{Z}^3/\mathbf{A}_0\mathbb{Z}^3 = \{0, \ldots, 2N-1\} \times \{0, \ldots, 2M-1\} \times \{0, \ldots, Q-1\}.$$

Let us define Y as in paper II:

$$Y(\mathbf{h}_1) = \sum_{\mathbf{x} \in \mathbf{A}_0\mathbb{Z}^3/\mathbf{A}_1\mathbb{Z}^3} f(\mathbf{x}) e_{\mathbf{A}}(\mathbf{h}_1, \mathbf{x}).$$

Then, from the symmetry-reduction formula of paper II [formula (15)], it follows that

$$\begin{aligned} F(\mathbf{h}_1) &= Y(\mathbf{h}_1) + e_{\mathbf{A}}(\mathbf{h}_1, -\mathbf{e}_3) Y(\mathbf{R}_\alpha^T \mathbf{h}_1) \\ F(\mathbf{h}_1 + \mathbf{A}_1\mathbf{e}_3^*) &= Y(\mathbf{h}_1) - e_{\mathbf{A}}(\mathbf{h}_1, -\mathbf{e}_3) Y(\mathbf{R}_\alpha^T \mathbf{h}_1). \end{aligned} \tag{8}$$

Now we can proceed to the second part: reducing translational symmetry. In our example, this means reducing the C-face centring, as described in §3.1. This procedure could be described in our table as:

Name	Vector $-\mathbf{b}$	Matrix $\mathbf{A}$	Algorithm
$C2$	$(0, 0, 0)$	$2\|x, 2\|y$	CCent.

Notice that now the matrix $\mathbf{A}_1$ from the previous stage plays the role of matrix $\mathbf{A}$ for the present stage. To avoid confusion, we will denote this matrix by $\mathbf{A}_{\rm CL}$:

$$\mathbf{A}_{\rm CL} = \begin{bmatrix} 2N & 0 & 0 \\ 0 & 2M & 0 \\ 0 & 0 & Q \end{bmatrix}.$$

Additionally, as explained in §3.1:

$$\tilde{\mathbf{A}}_0 = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \tilde{\mathbf{A}}_1 = \begin{bmatrix} N & 0 & 0 \\ 0 & M & 0 \\ 0 & 0 & Q \end{bmatrix}.$$

Note that $\mathbf{A}_{\rm CL} = \tilde{\mathbf{A}}_0\tilde{\mathbf{A}}_1$ (while $\mathbf{A} = \mathbf{A}_0\tilde{\mathbf{A}}_0\tilde{\mathbf{A}}_1$). Let $\tilde{\mathbf{h}} := \mathbf{h}_1$. Now, using these new matrices, we can decompose $\tilde{\mathbf{h}}$ according to formula (6). Now §3.1 yields that

$$Y(\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0 + \mathbf{e}_1^*) = 0 \quad \text{and} \quad Y(\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0 + \mathbf{e}_2^*) = 0,$$

where $\tilde{\mathbf{h}}_0 \in \mathbb{Z}^3/\tilde{\mathbf{A}}_1\mathbb{Z}^3$. It follows that the only points at which Y does not equal 0 are $\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0$ and $\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0 + \mathbf{e}_1^* + \mathbf{e}_2^*$ and

$$\begin{aligned} Y(\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0) &= F_1(\tilde{\mathbf{h}}_0) \\ Y(\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0 + \mathbf{e}_1^* + \mathbf{e}_2^*) &= F_2(\tilde{\mathbf{h}}_0), \end{aligned} \tag{9}$$

where F_1 and F_2 are Fourier transforms of functions:

$$\begin{aligned} f_1(\mathbf{x}) &= 2\{f(\mathbf{x}) + (T_y f)(\mathbf{x})\} \\ f_2(\mathbf{x}) &= 2e_{\mathbf{A}}((\mathbf{e}_1^* + \mathbf{e}_2^*), \mathbf{x})\{f(\mathbf{x}) - (T_y f)(\mathbf{x})\}, \end{aligned}$$

respectively. The asymmetric unit for the $C2$ group for this decomposition is depicted in Fig. 6. After substituting (8) into (9) and taking into account that $\mathbf{R}_\alpha^T$ commutes with $\mathbf{A}_0$ and $(\mathbf{A}_0^T)^{-1}\mathbf{A} = \tilde{\mathbf{A}}_0\tilde{\mathbf{A}}_1$, we obtain the final formulae:

$$
\begin{aligned}
F(\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0) &= F_1(\tilde{\mathbf{h}}_0) + e_{\mathbf{A}_{\rm CL}}(\tilde{\mathbf{h}}_0, \mathbf{e}_3)F_1(\mathbf{R}_\alpha^T\tilde{\mathbf{h}}_0)\\
F(\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0 + \mathbf{A}_1\mathbf{e}_3^*) &= F_1(\tilde{\mathbf{h}}_0) - e_{\mathbf{A}_{\rm CL}}(\tilde{\mathbf{h}}_0, \mathbf{e}_3)F_1(\mathbf{R}_\alpha^T\tilde{\mathbf{h}}_0)\\
F(\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0 + \mathbf{e}_1^* + \mathbf{e}_2^*) &= F_2(\tilde{\mathbf{h}}_0) + e_{\mathbf{A}_{\rm CL}}(\tilde{\mathbf{h}}_0, \mathbf{e}_3)F_2(\mathbf{R}_\alpha^T\tilde{\mathbf{h}}_0)\\
F(\tilde{\mathbf{A}}_0\tilde{\mathbf{h}}_0 + \mathbf{e}_1^* + \mathbf{e}_2^* + \mathbf{A}_1\mathbf{e}_3^*) &= F_2(\tilde{\mathbf{h}}_0) - e_{\mathbf{A}_{\rm CL}}(\tilde{\mathbf{h}}_0, \mathbf{e}_3)F_2(\mathbf{R}_\alpha^T\tilde{\mathbf{h}}_0).
\end{aligned}
$$

The formulae above, expressed in the coordinates h, k, l, read

$$
\begin{aligned}
F(2h, 2k, l) &= F_1(h, k, l) + \exp(-2\pi l/Q)\\
&\quad \times F_1(N-h, k, Q-l)\\
F(2h, 2k, l+Q) &= F_1(h, k, l) - \exp(-2\pi l/Q)\\
&\quad \times F_1(N-h, k, Q-l)\\
F(2h+1, 2k+1, l) &= F_2(h, k, l) + \exp(-2\pi l/Q)\\
&\quad \times F_2(N-h, k, Q-l)\\
F(2h+1, 2k+1, l+Q) &= F_2(h, k, l) - \exp(-2\pi l/Q)\\
&\quad \times F_2(N-h, k, Q-l),
\end{aligned}
$$

where $h = 0, 1, \ldots, N-1$ and $k = 0, 1, \ldots, M-1$ and $l = 0, 1, \ldots, Q-1$. The Fourier transform F equals zero at all other points of Γ^*, that is in points whose sum of h and k coordinates is odd.

5. Remarks on grid-size requirements

The residual translational symmetry left after the decomposition described in §§3 and 4 of paper II depends not only on the space group but also on the prime-factor decomposition of the number of grid points along x, y and z axes. A good example here is the plane group *cm*.

Let us switch to the grid coordinate system, described by

$$
\mathbf{A} = \begin{bmatrix} 2N & 0 \\ 0 & 2M \end{bmatrix} \quad \text{and} \quad \mathbf{b} = -\begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix},
$$

where N and M are positive integers.

The matrix describing our subgrid decomposition in this case reads

$$
\mathbf{A}_0 = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}.
$$

Let α denote the reflection with respect to the y axis and let β denote centring and let e denote the identity element of the symmetry group. Then, in the grid coordinate system, these symmetry operators are given by

$$
\begin{aligned}
\mathbf{R}_\alpha &= \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{t}_\alpha = \begin{bmatrix} -1 \\ 0 \end{bmatrix}\\
\mathbf{R}_\beta &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{t}_\beta = \begin{bmatrix} N \\ M \end{bmatrix}\\
\mathbf{R}_{\alpha\beta} &= \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{t}_{\alpha\beta} = \begin{bmatrix} N-1 \\ M \end{bmatrix}.
\end{aligned}
$$

Observe that

$$
\mathbf{t}_e = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}, \quad \mathbf{t}_\alpha = \begin{bmatrix} -1 \\ 0 \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 1 \\ 0 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}.
$$

However, it depends on the parity of N and M to which equivalence classes $\mathbf{t}_\beta$ and $\mathbf{t}_{\alpha\beta}$ belong. If N and M are both even, then

$$
\mathbf{t}_\beta = \begin{bmatrix} N \\ M \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}, \quad \mathbf{t}_{\alpha\beta} = \begin{bmatrix} N-1 \\ M \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 1 \\ 0 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}.
$$

If N is odd and M is even, then

$$
\mathbf{t}_\beta = \begin{bmatrix} N \\ M \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 1 \\ 0 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}, \quad \mathbf{t}_{\alpha\beta} = \begin{bmatrix} N-1 \\ M \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}.
$$

If N is even and M is odd, then

$$
\mathbf{t}_\beta = \begin{bmatrix} N \\ M \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 0 \\ 1 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}, \quad \mathbf{t}_{\alpha\beta} = \begin{bmatrix} N-1 \\ M \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 1 \\ 1 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}.
$$

If N and M are both odd, then

$$
\mathbf{t}_\beta = \begin{bmatrix} N \\ M \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 1 \\ 1 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}, \quad \mathbf{t}_{\alpha\beta} = \begin{bmatrix} N-1 \\ M \end{bmatrix} \in \left[\!\left[\begin{bmatrix} 0 \\ 1 \end{bmatrix} \right]\!\right]_{\mathbf{A}_0}.
$$

The next step depends on the parity of M. Let us first consider the case of M odd. Then Assumption 2 in §3 of paper II is fulfilled, that is the translational part of every symmetry operator belongs to a different equivalence class. This way, through the decomposition depicted in Fig. 7(*a*), a full reduction of symmetry is achieved.

Let us switch to the case of even M. To incorporate this condition into the matrix $\mathbf{A}$, we will write

$$
\mathbf{A} = \begin{bmatrix} 2N & 0 \\ 0 & 4M \end{bmatrix},
$$

where N and M are positive numbers. Observe that if we choose

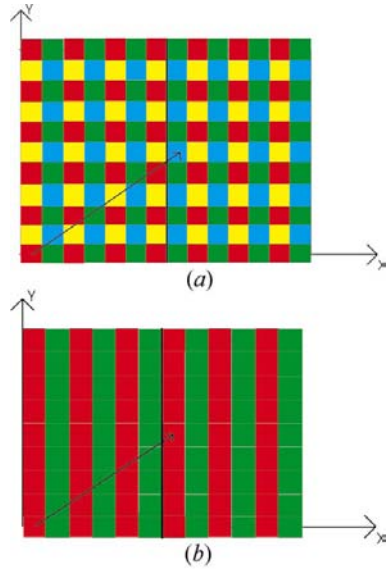

Figure 7
Subgrid decompositions for the *cm* plane group for different grid sizes. (*a*) The number of grid points along the x axis is divisible by 4, along y not divisible by 4, but still even. The non-primitive translation vector connects points in different subgrids. (*b*) The numbers of points along x and y axes are both divisible by 4. The centring vector in this case connects points from the same subgrid.

$$\mathbf{A}_0 = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \quad \text{and} \quad \mathbf{A}_1 = \begin{bmatrix} 2N & 0 \\ 0 & 2M \end{bmatrix},$$

then

$$\mathbf{t}_e = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \mathbf{t}_\alpha = \begin{bmatrix} -1 \\ 0 \end{bmatrix}, \quad \mathbf{t}_\beta = \begin{bmatrix} N \\ 2M \end{bmatrix}, \quad \mathbf{t}_{\alpha\beta} = \begin{bmatrix} N-1 \\ 2M \end{bmatrix}$$

and, since all second coordinates of these vectors are even,

$$\mathbf{t}_e,\ \mathbf{t}_\alpha,\ \mathbf{t}_\beta,\ \mathbf{t}_{\alpha\beta} \in \left[\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}.$$

This implies that no symmetry reduction is possible in this case. Therefore, we should choose another $\mathbf{A}_0$, for example

$$\mathbf{A}_0 = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}.$$

Suppose that N is odd. Then,

$$\mathbf{t}_e,\ \mathbf{t}_{\alpha\beta} \in \left[\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}, \quad \mathbf{t}_\alpha,\ \mathbf{t}_\beta \in \left[\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}.$$

After this decomposition, the residual symmetry will be given by the symmetry operator $-x+\frac{1}{2}, y+\frac{1}{2}$.

Now suppose that N is even. It follows that

$$\mathbf{t}_e,\ \mathbf{t}_\beta \in \left[\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}, \quad \mathbf{t}_\alpha,\ \mathbf{t}_{\alpha\beta} \in \left[\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}.$$

That is, we decompose the computational grid as shown in Fig. 7(*b*). Then there is a residual translational symmetry in every subgrid, the translation vector also depicted in this figure. One has to deal with translational symmetry, after reducing the non-translational symmetry first. This is done exactly as in the *C*-face centring (§3.1).

6. Discussion

There are different possible methods of dealing with centrings. One solution is to transform the coordinate system in such a way that the resulting lattice is primitive. Another is to use the multiplexing technique (Ten Eyck, 1973; Bricogne, 1993). The approach presented here is a different one. It is consistent with our philosophy of evaluating the crystallographic FFT, which is based on using a multidimensional Cooley–Tukey type of decomposition for symmetry reduction. The difference between our algorithms for treating centrings and other types of symmetry is that here the symmetry-specific step in the decomposition corresponds to Cooley–Tukey decomposition in the reciprocal space, as opposed to the real space in all other cases. The suitability of multidimensional Cooley–Tukey decomposition to treatment of centred lattices has also been suggested by Bricogne (1993).

We have shown how to reduce symmetry due to centring operators in crystallographic FFT calculations. We have also discussed how the presented algorithm can be combined with schemes dealing with other symmetry operators. The example of the *cm* group, discussed in the previous section, not only shows how the residual translational symmetry is affected by choosing grid size. It also shows that in order to cover all possible cases it would be necessary to list several combinations of algorithms (depending on grid size) for every space group. To avoid this, we decided to list in Appendix *A* only one case, the one that is most important in practice. It is the case in which N, M and Q can be divisible by arbitrarily high powers of 2. Therefore, sometimes, the full symmetry reduction can be achieved with assumptions weaker than those listed in Appendix *A*. However, for convenience sake, we prefer to impose the conditions from Appendix *A* and as a result to have only one[1] possible algorithm for each space group. This is very convenient, since it substantially simplifies the implementation of the crystallographic FFT. We emphasize that the conditions in question do not restrict the use of our algorithms in practice. To take full advantage of FFT (crystallographic or not), one always chooses their grid sizes to have as many small prime factors as possible, thus the requirement of the number of points in the asymmetric unit divisible by 4, 6, 8 or 16 is usually satisfied in the first place anyway.

In Appendix *B*, we list the conditions under which symmetry reduction can be achieved in one step, without special procedures for reducing translational symmetry. Unfortunately, these conditions are such that these algorithms are of little practical value.

APPENDIX *A*
Tables of algorithms

The tables below describe the set-up. Each row starts with the ITC number and name of the group (alternative descriptions of the same group are marked by alt). Following is the number of symmetry operators, denoted by $|G|$, it is approximately equal to the speedup achieved by using our algorithms. Then we list the vectors $-\mathbf{b}$ and the matrix $\mathbf{A}$ that define the grid coordinate system by (7). For example, the symbols $2|x, 2|y, 4|z$ given as a description of matrix $\mathbf{A}$ should be understood as follows:

$$\mathbf{A} = \begin{bmatrix} 2N & 0 & 0 \\ 0 & 2M & 0 \\ 0 & 0 & 4Q \end{bmatrix},$$

where N, M and Q are positive integers. There are various origins of requirements imposed on the entries of matrix $\mathbf{A}$. First, if our algorithm is to take every second point along the x, y and z axes, we first want to make sure that the number of points along these axes is even. In the case of the groups mentioned above, this requirement would lead to condition $2|x, 2|y, 2|z$. One of the reasons that we have additional conditions is that we want the computational grid to be invariant under the action of symmetry operators. We also want to have only one algorithm for every space group, so sometimes we imposed stricter than necessary (but not too strict for crystallographic applications) divisibility conditions to avoid considering several possibilities. This issue was

[1] Alternative algorithms, allowing for data points in special positions, can be constructed, too. They will be presented in paper IV.

discussed in §6. We emphasize that the restrictions on the size of the asymmetric unit we impose are far from significant. Often, we require simply that the asymmetric unit consists of an integer number of points. The strictest condition on the asymmetric unit in this paper is

Name	$\|G\|$	Matrix **A**	Algorithm
Fddd	32	$8\|x, 8\|y, 8\|z$	2x2y2z FCent.

This condition is still not restrictive. The *Fddd* group consists of 32 symmetry operators, so all we require is that the number of points in the asymmetric unit is divisible by 16 (this is partly due to the presence of the $-x+\frac{1}{4}, -y+\frac{1}{4}, -z+\frac{1}{4}$ operator in this crystallographic group). The last column of Table 1 contains a symbol of the algorithm used.

Symbol explanation: 2x: regular subgrid consisting of every second point along the x axis. 2x2y: regular subgrid consisting

Table 1
Algorithms for symmetry reduction for practical grid sizes; columns 1 and 2: crystallographic group number and symbol; column 3: number of elements; column 4: origin shift; column 5: minimal divisibility conditions for unit-cell sides; column 6: algorithm types for reducing non-translational and translational symmetry (see paper II and §3 above, respectively).

ITC No.	Name	$\|G\|$	Vector $-$**b**	Matrix **A**	Algorithm	
4 alt	$I2_1$†	4	$(\frac{1}{2}, 0, 0)$	$4\|x, 2\|y, 2\|z$	2x	ICent.
5	*C*121	4	$(0, 0, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2z	CCent.
5 alt	*C*21‡	4	$(0, 0, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2z	CCent.
5 alt	*A*2§	4	$(\frac{1}{2}, 0, 0)$	$2\|x, 2\|y, 2\|z$	2x	ACent.
8	*C*1*m*1	4	$(0, \frac{1}{2}, 0)$	$2\|x, 4\|y$	2y	CCent.
9	*C*1*c*1	4	$(0, \frac{1}{2}, 0)$	$2\|x, 4\|y, 2\|z$	2y	CCent.
12	$C12/m1$	8	$(0, \frac{1}{2}, \frac{1}{2})$	$2\|x, 4\|y, 2\|z$	2y2z	CCent.
15	$C12/c1$	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	CCent.
20	$C222_1$	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	CCent.
21	*C*222	8	$(0, \frac{1}{2}, \frac{1}{2})$	$2\|x, 4\|y, 2\|z$	2y2z	CCent.
22	*F*222	16	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	FCent.
23	*I*222	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ICent.
24	$I2_12_12_1$	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ICent.
35	*Cmm*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y$	2x2y	CCent.
36	$Cmc2_1$	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	CCent.
37	*Ccc*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	CCent.
38	*Amm*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$2\|x, 4\|y, 2\|z$	2x2y	ACent.
39	*Abm*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$2\|x, 4\|y, 2\|z$	2x2y	ACent.
40	*Ama*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ACent.
41	*Aba*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ACent.
42	*Fmm*2	16	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	FCent.
43	*Fdd*2	16	$(\frac{1}{2}, \frac{1}{2}, 0)$	$8\|x, 8\|y, 4\|z$	2x2y	FCent.
44	*Imm*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ICent.
45	*Iba*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ICent.
46	*Ima*2	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ICent.
63	*Cmcm*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	CCent.
64	*Cmca*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	CCent.
65	*Cmmm*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	2x2y2z	CCent.
66	*Cccm*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	2x2y2z	CCent.
67	*Cmma*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	2x2y2z	CCent.
68	*Ccca*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	CCent.
69	*Fmmm*	32	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	FCent.
70	*Fddd*	32	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$8\|x, 8\|y, 8\|z$	2x2y2z	FCent.
71	*Immm*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
72	*Ibam*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
73	*Ibca*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
74	*Imma*	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
79	*I*4	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ICent.
80	$I4_1$	8	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y	ICent.
82	$I\bar{4}$	8	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	2x2y	ICent.
87	$I4/m$	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
88	$I4_1/a$	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 8\|z$	2x2y2z	ICent.
97	*I*422	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
98	$I4_122$	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
119	$I\bar{4}m2$	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
120	$I\bar{4}c2$	16	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z	ICent.
146	*R*3	9	$(\frac{2}{3}, \frac{1}{3}, 0)$	$3\|x, 3\|y, 3\|z$	3(x+y)	RCent.

† $I2_1$ is the group defined by symmetry operators x, y, z; $-x, y+1/2, -z$; $x+1/2, y+1/2, z+1/2$; $-x+1/2, y, 1/2-z$. ‡ *C*21 is the group defined by symmetry operators x, y, z; $-x, y+1/2, -z$; $x+1/2, y+1/2, z$; $1/2-x, y, -z$. § *A*2 is the group defined by symmetry operators x, y, z; $-x, y+1/2, -z$; $x, y+1/2, z+1/2$; $-x, y, 1/2-z$.

Table 2
Algorithms for symmetry reduction for non-practical grid sizes; columns 1 and 2: crystallographic group number and symbol; column 3: origin shift; columns 4 and 5: divisibility conditions for unit-cell sides; column 6: algorithm type (see paper II).

ITC No.	Name	Vector $-$**b**	Matrix **A**	Conditions	Algorithm
4 alt	$I2_1$†	$(\frac{1}{2}, 0, \frac{1}{2})$	$4\|x, 2\|y, 2\|z$	*Q* odd	2x2z
5	*C*121	$(\frac{1}{2}, 0, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	*N* odd	2x2z
5 alt	*C*21‡	$(\frac{1}{2}, 0, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	*N* odd	2x2z
5 alt	*A*2§	$(\frac{1}{2}, 0, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	*Q* odd	2x2z
8	*C*1*m*1	$(0, \frac{1}{2}, 0)$	$2\|x, 2\|y$	*N* odd	2x2y
9	*C*1*c*1	$(0, \frac{1}{2}, 0)$	$2\|x, 2\|y, 2\|z$	*N* odd	2x2y
12	$C12/m1$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	*N* odd	2x2y2z
15	$C12/c1$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 2\|y, 2\|z$	*M* odd, *Q* odd	2x2y2z
20	$C222_1$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 2\|y, 2\|z$	*M* odd	2x2y2z
21	*C*222	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 2\|y, 2\|z$	*M* odd	2x2y2z
22	*F*222	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	*N* odd, *M* odd	4x4y
23	*I*222	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	*Q* odd	2x2y2z
24	$I2_12_12_1$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	*N* odd or *M* odd or *Q* odd	2x2y2z
35	*Cmm*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 2\|y$	*N* odd	4x2y
36	$Cmc2_1$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	*M* odd, *Q* odd	2x2y2z
37	*Ccc*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 2\|y, 2\|z$	*N* odd	4x2y
38	*Amm*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$2\|x, 2\|y, 2\|z$	*Q* odd	2x2y2z
39	*Abm*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$2\|x, 4\|y, 2\|z$	*M* odd	2x4y
40	*Ama*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	*M* odd	2x4y
41	*aba*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	*M* odd	2x4y
42	*Fmm*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 2\|z$	*N* odd, *M* odd	4x4y
43	*Fdd*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 4\|y, 4\|z$	*N* odd, *M* odd	4x4y
44	*Imm*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$2\|x, 2\|y, 2\|z$	*Q* odd	2x2y2z
45	*Iba*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 2\|y, 2\|z$	*N* odd	4x2y
46	*Ima*2	$(\frac{1}{2}, \frac{1}{2}, 0)$	$4\|x, 2\|y, 2\|z$	*Q* odd	2x2y2z
63	*Cmcm*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	*N* odd	4x2y2zy
64	*Cmca*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	*N* odd	4x2y2zy
65	*Cmmm*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 2\|y, 2\|z$	*N* odd	4x2y2zy
66	*Cccm*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 2\|y, 2\|z$	*N* odd	4x2y2zy
67	*Cmma*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	*N* odd	4x2y2zy
68	*Ccca*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	*N* odd	4x2y2zy
69	*Fmmm*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	*N* odd, *M* odd	4x4y2z
70	*Fddd*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 8\|z$	*N* odd, *M* odd	4x4y2z
71	*Immm*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 2\|y, 2\|z$	*N* odd	4x2y2zy
72	*Ibam*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 2\|y, 2\|z$	*N* odd	4x2y2zy
73	*Ibca*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	*N* odd	4x2y2zy
74	*Imma*	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 2\|z$	*N* odd	4x2y2zy
79	*I*4	$(\frac{1}{2}, \frac{1}{2}, 0)$	$2\|x, 2\|y, 2\|z$	*Q* odd	2x2y2z
80	$I4_1$	$(\frac{1}{2}, \frac{1}{2}, 0)$	$2\|x, 2\|y, 4\|z$	*Q* odd	2x4z
82	$I\bar{4}$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 2\|z$	*Q* odd	2x2y2z
87	$I4/m$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 4\|z$	*Q* odd	2x2y4z
88	$I4_1/a$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 4\|z$	*M* odd, *Q* odd	2x2y4z
97	*I*422	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 4\|z$	*Q* odd	2x2y4z
98	$I4_122$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$4\|x, 4\|y, 4\|z$	*Q* odd	2x2y4z
119	$I\bar{4}m2$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 4\|z$	*Q* odd	2x2y4z
120	$I\bar{4}c2$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$2\|x, 2\|y, 4\|z$	*Q* odd	2x2y4z
146	*R*3	$(\frac{2}{3}, \frac{1}{3}, 0)$	$3\|x, 3\|y, 3\|z$	*Q* not divisible by 3	3(x+y) 3z

† $I2_1$ is the group defined by symmetry operators x, y, z; $-x, y+1/2, -z$; $x+1/2, y+1/2, z+1/2$; $-x+1/2, y, 1/2-z$. ‡ *C*21 is the group defined by symmetry operators x, y, z; $-x, y+1/2, -z$; $x+1/2, y+1/2, z$; $1/2-x, y, -z$. § *A*2 is the group defined by symmetry operators x, y, z; $-x, y+1/2, -z$; $x, y+1/2, z+1/2$; $-x, y, 1/2-z$.

of every second point along x and y axes (discussed in §4.1 of paper II). 2x2y2z: regular subgrid consisting of every second point along x, y and z axes (see §4.2 of paper II). 3(x+y): subgrid of $x + y$ divisible by 3 (see paper I and §4.3 of paper II). ICent.: body centring (see §3.4). FCent.: all-face centring (see §3.3). ACent.: A-face centring (see §3.2). CCent.: C-face centring (see §3.1). RCent.: rhombohedral centring.

APPENDIX *B*
Tables of algorithms for non-practical grid sizes

Here we present examples of algorithms restricted by a maximal divisibility of unit-cell sizes. They are conceptually simpler than those in Appendix *A*. However, since the typical numbers of grid points in crystallographic data processing are divisible by 2^6 up to 2^{10}, we consider these algorithms non-practical. In other words, by dealing with such grid sizes the benefit of a somewhat simpler algorithm will be outweighed by loss in the efficiency of the *P*1 FFT, as was pointed out in the *Discussion*. Table 2 describes the set-up. The columns have the same meaning as in Appendix *A*, except for the new column listing additional conditions on integers N, M and Q, parameterizing matrix **A**.

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