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Crystallographic Fast Fourier Transforms*†

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This paper presents methods for incorporating crystallographic symmetry properties into complex Fourier transforms in a form particularly well suited for use with the Cooley–Tukey fast Fourier transform algorithm. The crystallographic transforms are expressed in terms of a small number of one-dimensional special cases. The algebra presented here has been used to write computer programs for both Fourier syntheses and Fourier inversions. Even for some quite large problems (7000 structure factors and 149000 grid points in the asymmetric unit) the rate-limiting step is output of the answers.

Introduction

The fast Fourier transform method has been widely available since 1965, but has not yet been used extensively for crystallographic work. This paper shows how crystallographic symmetry elements may be incorporated into fast Fourier transform algebra in a form particularly suited for machine computation. The use of these methods leads to large savings in computation time for Fourier transforms and enables one to write very efficient space-group specific Fourier-synthesis programs. The advantages of the fast Fourier transform are not as great in crystallographic computing as in other fields, but one may reasonably expect an improvement of an order of magnitude over a space-group specific trigonometric program and a much greater improvement over a general-purpose trigonometric program. The methods presented here are likely to be most useful for macromolecular structures and for direct methods of crystal-structure determination. (In the latter case the convolutions can be calculated very efficiently by Fourier methods.)

There are several reasons for the smaller gain in efficiency in crystallographic problems than in other fields by fast Fourier transform methods. The most striking advantage of the method is that the cost of replacing a sequence of N complex numbers with N Fourier coefficients is reduced from something proportional to the square of N to something proportional to $N \log N$; in crystallographic problems explicit advantage is always taken of the fact that there are far fewer structure factors than grid points. Thus the cost of a crystallographic Fourier transform, appropriately factored, goes up by a factor of 16 if both the grid interval and number of structure factors are doubled for each dimension, instead of going up by a factor of 64 as might be expected on an N^2 basis. The cost of the corresponding fast Fourier transform depends only on the size of the grid and therefore goes up only by a factor of 8. Since any given crystallographic transform is usually rather short – of the order of 50 to 100 points – the advantage of $N \log N$ over N^2 is not as strong as in time-series analysis, for example, where N may be several thousand or more. Finally, most of the generally available fast Fourier transform programs suffer from various practical defects, such as being restricted to the case where N is a power of two, or being written in machine code for some specific computer. These problems, plus the lack of symmetry, have inhibited widespread use of the method.

This paper shows that most of the objections can be met. Examination of the algebra of the fast Fourier transform has shown how nearly all symmetry elements can be fully exploited. Those which cannot be fully exploited are at least helpful. It has been emphasized elsewhere (Gentleman & Sande, 1966) that the method is not restricted to powers of two. Actual timings of programs written using the methods described here have shown that, on a medium-sized computer (an IBM 360/44), a protein electron-density map with 7000 unique structure factors and 149000 grid points in the asymmetric unit can be calculated faster than it can be written onto magnetic tape.

The methods presented here can also be used to invert electron-density maps to obtain structure factors. For every special form presented there is also a special form for the inverse transform. Given a reasonably cheap method for generating the desired electron-density map from a list of coordinates this may well be the method of choice when only structure factors are desired, as in Fourier refinement or direct methods of solving structures. Another potentially useful application for the structure-factor calculation is calculating structure factors for macromolecules, where the resolution is typically fairly low (between 2 and 3 Å) and the number of structure factors is very large.

This paper is in three parts. The first part describes the factoring of the Fourier transform, and borrows

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heavily from the work of Gentleman & Sande (1966). The second part shows how to incorporate one-dimensional phase relationships into the calculation of Fourier transforms. (Each such relationship is worth at least a factor of two in computation time and another factor of two in computer memory.) The third part shows how the symmetry properties of reciprocal space can be used, along with some of the properties of Fourier transforms listed in Table 1, to calculate three-dimensional Fourier transforms for selected space groups.

Notation

$R(t)$, $S(t)$, $X(t)$, $Y(t)$, $Z(t)$, $t=0, \ldots, N-1$ are sequences of (possibly) complex numbers. R, S, X, Y, and Z are to be considered as periodic modulo N, so that $X(-t)=X(N-t)$.

$X^*(t)$ is the complex conjugate of $X(t)$.

Re (X) is the real part of X.

Im (X) is the imaginary part of X.

$e(x)=\exp(-2\pi ix)$

$e(x)=1$ for any integer x

$e(a+b)=e(a)e(b)$

$e(1-x)=e(-x)$

$\mathbf{R(t)}$, $\mathbf{S(t)}$, $\mathbf{X(t)}$, $\mathbf{Y(t)}$, $\mathbf{Z(t)}$, $\mathbf{t}=0, \ldots, N-1$ are the finite discrete Fourier transforms of R, S, X, Y, Z defined as

$$\mathbf{X(t)}=\sum_{t=0}^{N-1} X(t)e(t\mathbf{t}/N)\,.$$

x, y, and z are fractional cell coordinates.

$F(h,k,l)$ is a (possibly) complex structure factor.

$\varphi(h,k,l)$ is the phase angle associated with $F(h,k,l)$.

$T_l(h,k,z)$ is the Fourier transform along l of $F(h,k,l)$.

Factoring the finite discrete Fourier transform

It can easily be seen from the definition of the finite discrete Fourier transform that the cost of replacing a sequence of N Fourier coefficients with their Fourier transforms is proportional to the square of N. Cooley & Tukey (1965) showed that if N has factors the Fourier transform may be computed as a series of shorter transforms, reducing the cost to something proportional to $N \log N$. A very clear description and discussion of the method is given by Gentleman & Sande (1966). The description of the factoring process given here is based on that of Gentleman & Sande.

Let $N=AB$. Then the expressions $aB+b$ and $a+bA$ will each generate all of the integers in the range $0 \le t < N$ when $a=0, \ldots, A-1$ and $b=0, \ldots, B-1$. If we let $t=aB+b$ and $\mathbf{t}=\mathbf{a}+\mathbf{b}A$ (a, $\mathbf{a}=0, \ldots, A-1$; b, $\mathbf{b}=0, \ldots, B-1$) the Fourier transform of $X(t)$ may be written as

$$\mathbf{X(t)}=\sum_{t=0}^{N-1} X(t)e(t\mathbf{t}/N)$$

$$\mathbf{X(a+bA)}=\sum_{b=0}^{B-1}\sum_{a=0}^{A-1} X(aB+b)e[(aB+b)(\mathbf{a}+\mathbf{b}A)/AB]\,. \quad (1)$$

The exponential may be expanded as

$$e[(aB+b)(\mathbf{a}+\mathbf{b}A)/AB]=e(a\mathbf{a}/A)e(a\mathbf{b})e(b\mathbf{a}/AB)e(b\mathbf{b}/B)$$
$$=e(a\mathbf{a}/A)e(b\mathbf{a}/AB)e(b\mathbf{b}/B)\,. \quad (2)$$

The transform is therefore

$$\mathbf{X(a+bA)}$$
$$=\sum_{b=0}^{B-1} e(b\mathbf{b}/B)\,[e(b\mathbf{a}/AB)\sum_{a=0}^{A-1} X(aB+b)e(a\mathbf{a}/A)]\,. \quad (3)$$

The inner sum is a Fourier transform of length A and the outer sum is a Fourier transform of length B. The cost of replacing $X(t)$ by its transform is now proportional to N times the sum of the factors of N, which is roughly proportional to $N \log N$.

It is often believed that the fast Fourier transform is restricted to the case where N is a power of 2. It can be seen from the above algebra that this is not true. Factors of 2 and 4 *are* very useful, because 2-point and 4-point Fourier transforms can be computed without using complex multiplication, but the method is not limited to this case.

A very good discussion of the problems of writing computer programs using equation (3) is given in the paper by Gentleman & Sande (1966). Those authors also give a useful table comparing properties of the infinite continuous Fourier transform and the finite discrete Fourier transform. Some of these properties are included in Table 1, along with others of interest for crystallographic computing. The two ways of factoring the Fourier transform by two are particularly important in the discussion that follows.

Table 1. *Useful properties of Fourier transforms*

(1) Linearity.

If
$$Z(t)=aX(t)+bY(t),$$
then
$$\mathbf{Z(t)}=a\mathbf{X(t)}+b\mathbf{Y(t)}.$$

(2) Inverse transform.
$$X(t)=[\sum_{t=0}^{N-1} \mathbf{X(t)}e(-t\mathbf{t}/N)]/N$$
$$=[\sum_{t=0}^{N-1} \mathbf{X}^*\mathbf{(t)}e(t\mathbf{t}/N)]^*/N,$$
that is, the inverse transform is the complex conjugate of the Fourier transform of the complex conjugate, scaled by N.

(3) Shifting theorem.
$$\sum_{t=0}^{N-1} X(t+h)e(t\mathbf{t}/N)=e(-h\mathbf{t}/N)\mathbf{X(t)},$$
that is, an origin shift in real space is a phase shift in reciprocal space, and *vice-versa*.

(4) Conjugate symmetry.
$$\sum_{t=0}^{N-1} X^*(t)e(t\mathbf{t})/N)=\mathbf{X}^*(N-\mathbf{t}),$$
that is, the Fourier transform of the complex conjugate is the complex conjugate of the mirror image of the Fourier transform.

Table 1 (*cont.*)

(5) Inversion symmetry.

$$\sum_{t=0}^{N-1} X(N-t)e(t\mathbf{t}/N)=\mathbf{X}(N-\mathbf{t}),$$

that is, the Fourier transform of the mirror image is the mirror image of the Fourier transform.

(6) Mirror symmetry and antisymmetry.

If

$$X(N-t)=X(t)$$

then

$$\mathbf{X}(N-\mathbf{t})=\mathbf{X}(\mathbf{t}).$$

If

$$X(N-t)=-X(t)$$

then

$$\mathbf{X}(N-\mathbf{t})=-\mathbf{X}(\mathbf{t}).$$

(7) Hermitian symmetry and antisymmetry.

If

$$X(N-t)=X^*(t)$$

then $\mathbf{X}(\mathbf{t})$ is real, and *vice-versa.*

If

$$X(N-t)=-X^*(t)$$

then $\mathbf{X}(\mathbf{t})$ is imaginary, and *vice-versa.*

(8) Periodicity and antiperiodicity.

If

$$X(t+N/2)=X(t)$$

then $\mathbf{X}(2\mathbf{t}+1)=0$, and *vice-versa.*

If

$$X(t+N/2)=-X(t)$$

then $\mathbf{X}(2\mathbf{t})=0$, and *vice-versa.*

(9) Convolution theorem.

$$\sum_{s=0}^{N-1} X(s)Y(t-s)=[\sum_{t=0}^{N-1}\mathbf{X}(\mathbf{t})\mathbf{Y}(\mathbf{t})e(-t\mathbf{t}/N)]/N$$
$$=[\sum_{t=0}^{N-1}\mathbf{X}^*(\mathbf{t})\mathbf{Y}^*(\mathbf{t})e(t\mathbf{t}/N)]^*/N,$$

that is, the convolution of X and Y is the inverse transform of the product of the Fourier transforms of X and Y.

(10) Factoring by 2.

Let $N=2A$; $t, \mathbf{t}=0, \ldots, A-1$.

Case I:

Let $R(t)=X(2t)$

and

$$S(t)=X(2t+1).$$

Then

$$\mathbf{X}(\mathbf{t})=\mathbf{R}(\mathbf{t})+e(\mathbf{t}/N)\mathbf{S}(\mathbf{t})$$

and

$$\mathbf{X}(\mathbf{t}+A)=\mathbf{R}(\mathbf{t})-e(\mathbf{t}/N)\mathbf{S}(\mathbf{t}).$$

Case II:

Let $R(t)=X(t)+X(t+A)$

and

$$S(t)=e(t/N)\,[X(t)-X(t+A)].$$

Then

$$\mathbf{X}(2\mathbf{t})=\mathbf{R}(\mathbf{t})$$

and

$$\mathbf{X}(2\mathbf{t}+1)=\mathbf{S}(\mathbf{t}).$$

(These are special cases of the factored Fourier transform derived from equation (3) by direct substitution.)

One-dimensional Fourier transforms with special properties

The distinguishing feature of crystallographic Fourier transforms is the high degree of symmetry involved. The symmetry is usually expressed in terms of complicated trigonometric formulae, as in *International Tables for Crystallography* (1952). These formulae tend to obscure the true symmetry of reciprocal space, which is best expressed in terms of point groups with colour symmetry, as shown by Bienenstock & Ewald (1962). When the point groups are examined it is found that there are a small number of types of special relationship between positive and negative values of the same reciprocal-space index in all of the monoclinic and orthorhombic space groups, and for a number of other space groups of higher symmetry. With a set of subroutines to handle these relationships and to use the Hermitian symmetry of reciprocal space one can use fast Fourier transform techniques *and* take full advantage of all of the crystallographic symmetry elements for these space groups.

In all of the special cases discussed below, N is assumed for convenience to be even, and $A=N/2$. The problem considered in each case is that of using only the unique information to calculate the unique portion of the Fourier transform, using an ordinary complex Fourier transform as the basic tool. Since all other forms are reduced to one-dimensional complex Fourier transforms the efficiency of the method depends critically on the efficiency with which such transforms can be calculated.

(*A*) *Hermitian symmetry and anti-symmetry*

It is frequently the case that $X(-t)=X^*(t)$. The Fourier transform consists of N real numbers; the unique portion of the data contains $A+1$ real numbers and $A-1$ imaginary numbers. [Both $X(0)$ and $X(A)$ are real.]

$$\text{Let } R(t)=X(t)+X(t+A)$$
$$=X(t)+X^*(A-t);$$

$$R(A-t)=X(A-t)+X(2A-t)$$
$$=X(A-t)+X^*(t):$$

$$S(t)=e(t/N)\,[X(t)-X(t+A)]$$
$$=e(t/N)\,[X(t)-X^*(A-t)];$$

and

$$S(A-t)=e(-t/N)\,[X(A-t)-X^*(t)]\,.$$

Then $\mathbf{R}(\mathbf{t})=\mathbf{X}(2\mathbf{t})$ and $\mathbf{S}(\mathbf{t})=\mathbf{X}(2\mathbf{t}+1)$. If we let

$$Y(t)=R(t)+iS(t)$$

then

$$\mathbf{Y}(\mathbf{t})=\mathbf{X}(2\mathbf{t})+i\mathbf{X}(2\mathbf{t}+1)$$

because of the linearity property. Thus the Fourier transform of Y has the desired transform of X in its real and imaginary parts. Note that the sequence $Y(t)$

may be formed in one pass through the data working in from each end, overwriting the original data. Thus the transform may be calculated in place without using scratch storage.

The processing of a Hermitian antisymmetric sequence differs only in the sign of the complex conjugate terms and in the fact that the resulting transform is imaginary instead of real. The even terms will be found in the imaginary part of **Y** and the odd terms will be found *negated* in the real part of **Y**.

(*B*) *Real and imaginary data*

As might be expected, this problem is just the inverse of the previous one.

Let

$$R(t)=X(2t);$$

$$S(t)=X(2t+1);$$

and

$$Y(t)=R(t)+iS(t)\,.$$

Then $\mathbf{Y}=\mathbf{R}+i\mathbf{S}$. If X is real, **R** and **S** are Hermitian symmetric modulo A. The Fourier transforms of R and S may be recovered from that of Y by conjugate symmetry and recombined to give the unique part of the Fourier transform of X.

$$\mathrm{Re}\,[\mathbf{Y(t)}]=\mathrm{Re}\,[\mathbf{R(t)}]-\mathrm{Im}\,[\mathbf{S(t)}]$$

$$\mathrm{Re}\,[\mathbf{Y}(A-\mathbf{t})]=\mathrm{Re}\,[\mathbf{R(t)}]+\mathrm{Im}\,[\mathbf{S(t)}]$$

$$\mathrm{Im}\,[\mathbf{Y(t)}]=\mathrm{Re}\,[\mathbf{S(t)}]+\mathrm{Im}\,[\mathbf{R(t)}]$$

$$\mathrm{Im}\,[\mathbf{Y}(A-\mathbf{t})]=\mathrm{Re}\,[\mathbf{S(t)}]-\mathrm{Im}\,[\mathbf{R(t)}]$$

$$\mathbf{X(t)}=\mathbf{R(t)}+e(\mathbf{t}/N)\mathbf{S(t)}$$

$$\mathbf{X}(A-\mathbf{t})=\mathbf{R}(A-\mathbf{t})+e[(A-\mathbf{t})/N]\mathbf{S}(A-\mathbf{t})$$

$$=\mathbf{R}^*(\mathbf{t})-e(-\mathbf{t}/N)\mathbf{S}^*(\mathbf{t})\,.$$

The treatment of imaginary data differs only in minor details. The sequences **R** and **S** are Hermitian antisymmetric instead of symmetric; this and the multiplication by i will change some of the signs.

(*C*) *Alternating Hermitian symmetric and antisymmetric data*

A screw diad passing through the origin produces relationships of the form

$$X(-t)=(-1)^tX^*(t)\,.$$

Given only half of the structure factors we wish to compute half of the Fourier transform.

Let

$$R(t)=X(2t)\,.$$

$$S(t)=X(2t+1)\,,$$

and

$$Y(t)=R(t)+iS(t)\,.$$

Then

$$\mathbf{Y(t)}=\mathbf{R(t)}+i\mathbf{S(t)}$$

and

$$\mathbf{X(t)}=\mathbf{R(t)}+e(\mathbf{t}/N)\mathbf{S(t)}\,.$$

The Fourier transforms of R and S may be recovered from **Y** by using the fact that **R**(**t**) is real and $e(\mathbf{t}/N)\mathbf{S}(\mathbf{t})$ is imaginary. This works for all values of **t** except 0. **S**(0) can be computed and saved while Y is being formed; it is merely the sum of the imaginary parts of the structure factors for which $t=2n+1$. The sequence $Y(t)$ can be formed in place overwriting $X(t)$, but not in natural order. The most convenient order for forming $Y(t)$ is

$$Y(t)=X(2t)+iX(2t+1)$$
$$Y(A-t-1)=X^*(2t+2)-iX^*(2t+1)$$

where $X(2t)$ is overwritten by $Y(t)$ and $X(2t+1)$ is overwritten by $Y(A-t-1)$. Re-ordering Y before calculating the transform is a simple matter.

(*D*) *Symmetric and anti-symmetric data*

For symmetric data with N even we have $X(t)=X(N-t)$, with both $X(0)$ and $X(A)$ being unique. This gives $A+1$ unique numbers.

Let

$$R(t)=X(2t)\,,$$

$$S(t)=X(2t+1)\,,$$

and

$$Y(t)=R(t)+S(t)\,.$$

The sequence X may be overwritten by Y in a manner analogous to that described for the case of alternating Hermitian symmetry and antisymmetry, that is

$$Y(t)=X(2t)+X(2t+1);$$
$$Y(A-t-1)=X(2t+2)+X(2t+1);$$

$X(2t)$ is overwritten by $Y(t)$ and $X(2t+1)$ is overwritten by $Y(A-t-1)$. Then

$$\mathbf{X(t)}=\mathbf{R(t)}+e(\mathbf{t}/N)\mathbf{S(t)}$$

and

$$\mathbf{X}(\mathbf{t}+A)=\mathbf{R(t)}-e(\mathbf{t}/N)\mathbf{S(t)}\,.$$

R and **R** are both symmetric modulo A; **X** is symmetric modulo N. Thus we have

$$\mathbf{X}(N-\mathbf{t})=\mathbf{X}(2A-\mathbf{t})$$
$$=\mathbf{R}(A-\mathbf{t})-e[(A-\mathbf{t})/N]\mathbf{S}(A-\mathbf{t})$$
$$=\mathbf{R(t)}+e(-\mathbf{t}/N)\mathbf{S}(A-\mathbf{t})\,,$$

which when combined with the expression for **X**(**t**) implies that

$$\mathbf{S}(A-\mathbf{t})=e(2\mathbf{t}/N)\mathbf{S(t)}\,.$$

Since $\mathbf{Y}=\mathbf{R}+\mathbf{S}$,

$$\mathbf{Y}(A-\mathbf{t})-\mathbf{Y(t)}=\mathbf{S}(A-\mathbf{t})-\mathbf{S(t)}$$
$$=[e(2\mathbf{t}/N)-1]\mathbf{S(t)}\,.$$

Thus the Fourier transform of Y may be separated into **R** and **S**, which can be combined to give the desired half of the Fourier transform of X. This is valid for all points except **X**(0) and **X**(A). For these points we have

$$\mathbf{X}(0)=\mathbf{R}(0)+\mathbf{S}(0)$$

and

$$\mathbf{X}(A)=\mathbf{R}(0)-\mathbf{S}(0)\,.$$

If X is overwritten with Y the value of **S**(0) may be computed while Y is being formed and stored in the location originally occupied by $X(A)$, which is not used for Y. Then

$$\mathbf{X}(0)=\mathbf{Y}(0)$$

and

$$\mathbf{X}(A)=\mathbf{Y}(0)-2\mathbf{S}(0)\,.$$

The treatment of an antisymmetric sequence is the same as that for a symmetric sequence, except that

$$Y(A-t-1)=-X(2t+2)-X(2t+1);$$

$$\mathbf{R}(A-\mathbf{t})=-\mathbf{R}(\mathbf{t});$$

$$\mathbf{S}(A-\mathbf{t})=-e(2\mathbf{t}/N)\mathbf{S}(\mathbf{t});$$

and

$$\mathbf{Y}(A-\mathbf{t})+\mathbf{Y}(\mathbf{t})=\mathbf{S}(\mathbf{t})\,[1-e(2\mathbf{t}/N)]\,.$$

Symmetric data are frequently real rather than complex. In this case Y is real and **Y** is Hermitian symmetric modulo A. The Fourier transform of Y may be calculated using the methods described previously. The Fourier transform of R (which is real and symmetric modulo A) may be separated from the Fourier transform of S (which is Hermitian symmetric modulo A) by using the fact that $e(\mathbf{t}/N)\mathbf{S}(\mathbf{t})$ is *real*. Then

$$\mathbf{X}(\mathbf{t})=\mathbf{R}(\mathbf{t})+e(\mathbf{t}/N)\mathbf{S}(\mathbf{t})$$

and

$$\mathbf{X}(A-\mathbf{t})=\mathbf{R}(\mathbf{t})-e(\mathbf{t}/N)\mathbf{S}(\mathbf{t})\,.$$

These two real numbers can be stored in the real and imaginary parts of **Y**(**t**), and thus the whole calculation can be done in place.

Three-dimensional Fourier transforms with symmetry

The symmetry properties of reciprocal space are best expressed in terms of complex point groups with colour symmetry, as was shown by Bienenstock & Ewald (1962). Their paper describes methods for deriving the point groups corresponding to each of the 230 space groups. Each such point group is composed of operators of the form

$$\begin{pmatrix} h' \\ k' \\ l' \\ \varphi' \end{pmatrix} = \begin{pmatrix} & & & 0 \\ & \mathsf{R} & & 0 \\ & & & 0 \\ a & b & c & 1 \end{pmatrix} \begin{pmatrix} h \\ k \\ l \\ \varphi \end{pmatrix},$$

where R is a point operator relating two points in reciprocal space which have identical amplitudes and φ is a phase angle associated with that point. The arithmetic involving φ is always to be taken as periodic modulo 2π. The operator (-1), which is simply an expression of Friedel's law, is also a member of every such point group. Constraints on the coefficients in the bottom row of the operator are obtained by applying the operator to itself until the identity operator is achieved. Those coefficients which are unconstrained depend on the origin in real space. As an example, consider a twofold rotation axis parallel to **c***. The corresponding operator is

$$\begin{matrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ a & b & c & 1\,. \end{matrix}$$

Therefore $2c=0$ modulo 2π. If $c=0$, we have a diad in real space; if $c=\pi$ we have a screw diad. A list of a number of operators and derived constraints is given in Table 2; some more examples are given in the discussion for specific space groups.

Table 2. *Reciprocal space symmetry operators*

(1) Inversion centre

-1	0	0	0	$\varphi(h,k,l)=-(ha+kb+lc)/2$
0	-1	0	0	
0	0	-1	0	
a	b	c	1	

(2) Twofold axis

-1	0	0	0	$2c=0$ modulo 2π
0	-1	0	0	for 2 $c=0$
0	0	1	0	for 2_1 $c=\pi$
a	b	c	1	

(3) Threefold axis (on 60 coordinate axes)

-1	-1	0	0	$3c=0$ modulo 2π
1	0	0	0	for 3 $c=0$
0	0	1	0	for 3_1 $c=2\pi/3$
a	b	c	1	for 3_2 $c=4\pi/3$

(4) Fourfold axis

0	-1	0	0	$4c=0$ modulo 2π
1	0	0	0	for 4 $c=0$
0	0	1	0	for 4_1 $c=\pi/2$
a	b	c	1	for 4_2 $c=\pi$
				for 4_3 $c=3\pi/2$

(5) Sixfold axis

				$6c=0$ modulo 2π
0	-1	0	0	for 6 $c=0$
1	1	0	0	for 6_1 $c=\pi/3$
0	0	1	0	for 6_2 $c=2\pi/3$
a	b	c	1	for 6_3 $c=\pi$
				for 6_4 $c=4\pi/3$
				for 6_5 $c=5\pi/3$

(6) Plane of symmetry

				$2a=0$ modulo 2π
1	0	0	0	$2b=0$ modulo 2π
0	1	0	0	$a=0$ $b=0$ for m
0	0	-1	0	$a=\pi$ $b=0$ for a-glide
a	b	c	1	$a=0$ $b=\pi$ for b-glide
				$a=\pi$ $b=\pi$ for n-glide

Six of the seven crystal systems are discussed below; the cubic system is too complex for this paper. In the discussion that follows a space group is considered 'solved' when only a unique set of structure factors is required to calculate a crystallographic asymmetric unit, without calculating unnecessary intermediate results. A space group is 'nearly solved' if more than an asymmetric unit must be calculated or if redundant intermediate results must be computed. All of the triclinic, monoclinic, and orthorhombic space groups can be solved. Most of those tetragonal, trigonal, and hexagonal space groups which involve screw axes can be solved. Those space groups in which the boundaries of the asymmetric unit are not parallel to the edges of the unit cell cannot be solved but can be nearly solved. Regardless of the space group, the last Fourier tansform must be Hermitian symmetric because the results must be real.

(*A*) *Triclinic system*

Both space groups in this system are trivial. The only special symmetry is that the structure factors for $P\bar{1}$ are real, so the first transform gives results for half the cell.

(*B*) *Monoclinic system*

Most of the monoclinic space groups are simple examples of the special transforms described previously. Two space groups will be considered in detail to illustrate some points of special interest. The second setting will be used, and the unique set of structure factors taken as all h, $k \geq 0$, and $l \geq 0$.

(1) $C2$

The diad along **b*** plus the Hermitian inversion centre makes the Fourier transform along k Hermitian symmetric, giving real results for the whole axis from half the structure factors. The centred lattice introduces systematic absences for $h+k=2n+1$, so from the periodicity and antiperiodicity properties in Table 1 it can be seen that for $h=2n+1$ the transform will be periodic modulo $N/2$ and for $h=2n$ it will be antiperiodic. We can therefore add the h-even and h-odd sets of structure factors and recover the intermediate results by

$$T_k(h',y,l)=T_k(2h+1,y,l)+T_k(2h,y,l)$$
$$T_k(h',y+\tfrac{1}{2},l)=T_k(2h+1,y,l)-T_k(2h,y,l)$$

where $h'=h/2$ truncated to an integer value. Thus we have real intermediate results for all h, $0 \leq y \leq \frac{1}{2}$, and $l \geq 0$; the transforms on h and l give half x, half y, all z as an asymmetric unit. This method of treating centred lattices is generally applicable and no further examples will be given.

(2) $P2_1/c$

This space group has been selected to illustrate the conversion from a symmetry element at the origin to another more favourable case. The origin for this space group is taken as the centre of symmetry, so the structure factors are all real. Because of the glide plane and the screw diad the relationship along k is given by

$$F(h,-k,l)=(-1)^{k+l}F(h,k,l)\,.$$

The alternating symmetry and antisymmetry along k is complicated by the dependence on the parity of l. If we let $l'=l/2$ truncated to an integer, we may form

$$X(h,k,l')=F(h,k,2l')+iF(h,k,2l'+1)$$

which has alternating Hermitian symmetry and antisymmetry along k. The Fourier transform of X along k can be separated because it is the sum of a Hermitian symmetric sequence and a Hermitian anti-symmetric sequence. Thus

$$T_k(h,y,2l')=[\mathbf{X}(h,\tfrac{1}{2}-y,l')+\mathbf{X}(h,y,l')]/2$$

and

$$T_k(h,y,2l'+1)=[\mathbf{X}(h,\tfrac{1}{2}-y,l')-\mathbf{X}(h,y,l')]/2i\,.$$

Transforming on h and l then gives as an asymmetric unit that portion of the cell lying between $y=0$ and $y=\frac{1}{4}$.

The relationship between the method just presented and shifting the screw diad at $c/4$ to the origin is fairly obvious. By the shifting theorem (Table 1) we would have

$$F'(h,k,l)=e(-\tfrac{1}{4})F(h,k,l)$$

which would make the l-odd structure factors imaginary. The real and imaginary sequences along k each satisfy the screw diad phase relationships, that is,

$$F'(h,-k,l)=(-1)^kF'^*(h,k,l)$$

and can be added pairwise to form a sequence which has exactly the same symmetry along k as X. The sign reversals for $l=2$ modulo 4 and $l=3$ modulo 4 do not affect the relationship between positive and negative values of k. Thus the method given here for transforming this space group is very similar to shifting the screw diad to the origin, transforming, and shifting it back to $c/4$.

(*C*) *Orthorhombic system*

In this crystal system the unique set of structure factors will be taken as h, k, and l all ≥ 0. Because of the *mmm* symmetry of the diffraction pattern it is always possible to derive phase relationships along each axis. The first transform therefore seldom presents problems. The second transform may require transposition of intermediate results, in the case where twofold axes are involved instead of planes of symmetry. In the discussions that follow the first transform will be along l and the second transform along whichever axis is most convenient – usually k.

(1) $P222$

In this space group all axes are equivalent and Hermitian symmetric. Therefore we can calculate $T_l(h,k,z)$

(which is real) for all z. Since

$$\varphi(h,-k,l)=-\varphi(h,k,l)\,.$$
$$T_l(h,-k,z)=T_l^*(h,k,-z)=T_l(h,k,-z)\,.$$

By transposing intermediate results we can complete the transform to compute all x, half y, and half z as an asymmetric unit.

(2) $P2_12_12_1$

This space group is complicated by the fact that none of the symmetry elements pass through the origin. The point group operators are

$$\begin{matrix}-1&0&0&0\\0&-1&0&0\\0&0&1&0\\\pi&0&\pi&1\end{matrix}\quad\text{and}\quad\begin{matrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\\pi&\pi&0&1\end{matrix}$$

where the origin-dependent parameters are chosen to make all axes equivalent. Therefore

$$\varphi(h,k,-l)=(h+l)\pi-\varphi(h,k,l)$$

and

$$\varphi(h,-k,l)=(h+k)\pi+\varphi(h,k,-l)\,.$$

Examining first the relationships along l we see that for h even we have the same phase relationships as for a screw diad through the origin. For h odd, the phase relationships are reversed. By the linearity property we may multiply the h-odd structure factors by i, transform, and divide by i to recover the desired transform. Multiplication of the h-odd structure factors by i gives them the same phase relationships as the h-even structure factors. We may therefore calculate $T_l(h,k,z)$ for half z. Examination of the phase relationships along the k axis shows that

$$F(h,-k,l)=(-1)^{h+k}F(h,k,-l)\,.$$

Therefore we may complete the transform by

$$T_l(h,-k,z)=(-1)^{h+k}T_l(h,k,-z)$$
$$=(-1)^kT_l^*(h,k,\tfrac{1}{2}-z)$$

because

$$T_l(h,k,-z)=(-1)^hT_l^*(h,k,\tfrac{1}{2}-z)\,.$$

This gives all x, all y, and one fourth z as an asymmetric unit.

(3) *Pbca*

This space group has an inversion centre at the origin and three mutually perpendicular glide planes. The structure factors are real and the following relationships are easily derived.

$$F(h,k,-l)=(-1)^{h+l}F(h,k,l)\,,$$
$$F(h,-k,l)=(-1)^{k+l}F(h,k,l)\,,$$
$$F(-h,k,l)=(-1)^{h+k}F(h,k,l)\,,$$

and

$$F(h,-k,l)=(-1)^{h+k}F(h,k,-l)\,.$$

The Fourier transform along l can be calculated in the same manner as that along k for $P2_1/c$, giving complex intermediate results for one quarter of the z axis. To complete an asymmetric unit we need $\frac{1}{2}y$ and all x. From the last structure-factor relationship and the fact that the structure factors were initially real we can see that

$$T_l(h,-k,z)=(-1)^{h+k}T_l(h,k,-z)$$
$$=(-1)^{h+k}T_l^*(h,k,z)$$

which can be dealt with by multiplication of the h odd intermediate results by i, transforming as along a screw diad, and dividing the h-odd results by i. In fact, the intermediate results for the transform along l are recoverable directly in a form multiplied by i for h odd, which saves one stage of multiplication and division by i.

(*D*) *Tetragonal system*

The tetragonal system cannot be solved completely. A fourfold rotation axis can only be treated as a diad, although some economy is possible by expanding the intermediate results rather than the structure factors. Those tetragonal space groups with triangular asymmetric units (*e.g.* $P4/mmm$) can only be nearly solved as well, because the fast Fourier transform method is inherently incapable of calculating a triangular asymmetric unit. Those space groups corresponding to Laue symmetry $4/m$ are basically like the monoclinic space groups. Therefore only the fourfold aspects will be considered. The unique set of structure factors will be taken as h, k, and l all ≥ 0. Those space groups with Laue symmetry $4/mmm$ are basically like the orthorhombic system; the unique set of structure factors will be taken as $0\leq h$, $0\leq k\leq h$, and $0\leq 1$.

(1) $P4_1$, $P4_2$, *and* $P4_3$

From Table 2 we can see that the constraints for these space groups are all of the form

$$\varphi(-k,h,l)=\varphi(h,k,l)+nl\pi/2$$

which simply means an origin shift after transforming on l. For $P4_1$ and $P4_3$ the phase relationships along l are the same as those for a screw diad; for $P4_2$ they are the same as for a diad. After transformation along l the intermediate results may be transposed as

$$T_l(-k,h,z)=T_l(h,k,z+\tfrac{1}{4})\ (P4_1)\,,$$
$$T_l(-k,h,z)=T_l(h,k,z+\tfrac{1}{2})\ (P4_2)\,,$$
$$T_l(-k,h,z)=T_l^*(h,k,z+\tfrac{1}{4})\ (P4_3)\,.$$

The intermediate results for $P4_2$ are real. In each case transforming on h, then k gives an asymmetric unit.

(2) $P4_12_12$ *and* $P4_32_12$

The screw tetrad permits these enantiomorphic space groups to be completely solved. The desired phase relationships are generated from the diagonal diad

through the origin and the screw tetrad, that is

$$\begin{matrix}0&1&0&0\\1&0&0&0\\0&0&-1&0\\0&0&0&1\end{matrix}\quad\text{and}\quad\begin{matrix}0&-1&0&0\\1&0&0&0\\0&0&1&0\\a&b&\pi/2&1\end{matrix}$$

(The example is $P4_12_12$; the corresponding relations for $P4_32_12$ are derived in exactly the same manner.) The parameters a and b are determined by noting that application of the 4_1 twice must be equivalent to a 2_1 through the origin; therefore $b+a=0$ and $b-a=0$. Since the 4_1 does not pass through the origin we have $a=b=\pi$. From these two operators and the Hermitian inversion operator we may derive the following phase relationships.

$$\varphi(h,k,-l)=l\pi-\varphi(h,k,l)$$
$$\varphi(k,h,l)=\varphi(h,k,-l)$$
$$\varphi(-h,k,l)=(h+k)\pi-l\pi/2-\varphi(h,k,l)$$
$$\varphi(-k,h,l)=(h+k)\pi+l\pi/2+\varphi(h,k,l)\,.$$

We may therefore transform along l as though it were a 2_1 axis. The results may then be transposed to give

$$T_l(k,h,z)=T_l^*(h,k,\tfrac{1}{2}-z)$$
$$T_l(-h,k,z)=(-1)^{h+k}T_l^*(h,k,\tfrac{1}{4}-z)$$
$$T_l(-k,h,z)=(-1)^{h+k}T_l(h,k,\tfrac{1}{4}+z)$$

for $0\le z\le\frac{1}{8}$. The transforms on h and k can then be calculated to give one eighth of the cell along z as an asymmetric unit.

(*E*) *Trigonal and rhombohedral systems*

Those trigonal space groups conventionally indexed on rhombohedral axes cannot be economically treated on such axes by fast Fourier transform methods because there are no one-dimensional relationships. The choice of a rhombohedral cell is made on the grounds that it has one third the volume of the trigonal cell. It is a very simple matter to index the cell on trigonal axes and only compute one third of the cell volume by factoring the Fourier transform by three. Factoring by three gives (with $A=N/3$)

$$\mathbf{X}(\mathbf{t})=\sum_{t=0}^{A-1}X(3t)e(t\mathbf{t}/A)+e(\mathbf{t}/N)\sum_{t=0}^{A-1}X(3t+1)e(t\mathbf{t}/A)+e(2\mathbf{t}/N)\sum_{t=0}^{A-1}X(3t+2)e(t\mathbf{t}/A)$$

$$\mathbf{X}(\mathbf{t}+A)=\sum_{t=0}^{A-1}X(3t)e(t\mathbf{t}/A)+e(\tfrac{1}{3})e(\mathbf{t}/N)\sum_{t=0}^{A-1}X(3t+1)e(t\mathbf{t}/A)+e(\tfrac{2}{3})e(2\mathbf{t}/N)\sum_{t=0}^{A-1}X(3t+2)e(t\mathbf{t}/A)$$

$$\mathbf{X}(\mathbf{t}+2A)=\sum_{t=0}^{A-1}X(3t)e(t\mathbf{t}/A)+e(\tfrac{2}{3})e(\mathbf{t}/N)\sum_{t=0}^{A-1}X(3t+1)e(t\mathbf{t}/A)+e(\tfrac{1}{3})e(2\mathbf{t}/N)\sum_{t=0}^{A-1}X(3t+2)e(t\mathbf{t}/A)$$

where $\mathbf{t}=0,\ldots,A-1$.

Because of the equivalent positions at $(0,0,0)$, $(\frac{1}{3},\frac{2}{3},\frac{2}{3})$, and $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ there are systematic absences unless $k-h+l=3n$. Therefore, for the transform on l, only one of the three summations will be non-zero for any given value of h and k. There is thus no disadvantage in considering all trigonal space groups on trigonal axes.

The combination of threefold symmetry and Friedel's law means that only one sixth of reciprocal space need be specified as a unique set of structure factors. Since the reciprocal axes $\mathbf{a}^*$ and $\mathbf{b}^*$ are at an angle of sixty degrees and there are no convenient one-dimensional relationships along l, the unique set will be taken as h and $k\ge0$ and all l. Additional symmetry elements are of course helpful. An inversion centre reduces the computation by making the transform along l real. Planes of symmetry and diads reduce the computation by decreasing the unique set of structure factors from h and $k\ge0$ to $h\ge0$ and $0\le k\le h$.

(1) *P*3, *R*3, $P3_1$, *and* $P3_2$

In all of these space groups the Fourier transform along l is complex and has no special properties except the factoring by three for *R*3. The threefold rotation operator on hexagonal axes will carry the results from (h,k) to $(-h-k,h)$. To fill in the remaining third of the requisite intermediate results we may use the fact (true for all space groups) that

$$T_l(-h,-k,z)=T_l^*(h,k,z)$$

which is simply a statement that the final transform is real. The transposition relations for *P*3 and *R*3 (which can only be nearly solved) are

$$T_l(-h-k,h,z)=T_l(h,k,z)$$
$$T_l(-k,h+k,z)=T_l^*(h,k,z)$$

which completes the transform. The transposition relations for $P3_1$ and $P3_2$ (which can be solved) are

$$T_l(-h-k,h,z)=T_l(h,k,z+\tfrac{1}{3})\ (P3_1)$$
$$T_l(-k,h+k,z)=T_l^*(h,k,z+\tfrac{2}{3})\ (P3_1)$$
$$T_l(-h-k,h,z)=T_l(h,k,z+\tfrac{2}{3})\ (P3_2)$$
$$T_l(-k,h+k,z)=T_l^*(h,k,z+\tfrac{1}{3})\ (P3_2)$$

for $0\le z<\frac{1}{3}$.

(2) *$P3_112$ and $P3_121$*

These space groups are chosen to illustrate an important point about trigonal space groups with extra symmetry elements. The orientation of the diad in the transform is preserved, but the axes of the coordinate system have been altered. Thus the diad makes an angle of thirty degrees with **a*** in $P3_121$ but is along **a*** in $P3_112$. The point operator for the diad in $P3_112$ is

$$\begin{matrix} 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{matrix}$$

which can be combined with the operator for a 3_1 axis and a Hermitian inversion centre to obtain the relationship

$$\varphi(k,h,l) = -(2\pi/3)1 - \varphi(h,k,l)$$

which in turn gives

$$T_l(k,h,z) = T_l^*(h,k,\tfrac{1}{3}-z)\,.$$

This can be combined with the transposition relationships already given for $P3_1$ to fill in all h, $+k$, $0 \le z < \frac{1}{6}$, from which an asymmetric unit can be calculated. For $P3_121$ the twofold operator is

$$\begin{matrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{matrix}$$

which gives immediately

$$\varphi(k,h,l) = \varphi(h,k,-l)$$

and

$$T_l(k,h,z) = T_l(h,k,-z)$$

which again can be combined with the 3_1 relations to give an asymmetric unit.

(F) Hexagonal system

As would be expected the hexagonal system is very similar to the trigonal system in its transformation properties. The twofold component of the hexads reduces the number of structure factors required by a factor of two; only the positive half of l is required. A pure sixfold rotation axis can only be utilized as a diad, but all of the sixfold screw axes except 6_3 can be solved. (A 6_3 screw cannot be solved because the asymmetric unit is not favourable.) As an example of a fairly complicated hexagonal space group $P6_122$ will be used. The operator for the 6_1 axis is given in Table 2; the diad is given by

$$\begin{matrix} 1 & 0 & 0 & 0 \\ -1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1\,. \end{matrix}$$

From these operators we may derive the following phase relationships.

$$\begin{aligned} \varphi(h,k,-l) &= l\pi - \varphi(h,k,l) \\ \varphi(k,h,l) &= -l\pi/3 - \varphi(h,k,l) \\ \varphi(-k,h+k,l) &= l\pi/3 + \varphi(h,k,l) \\ \varphi(-h-k,k,l) &= l\pi/3 - \varphi(h,k,l) \\ \varphi(-h-k,h,l) &= 2l\pi/3 + \varphi(h,k,l) \\ \varphi(-h,h+k,l) &= -\varphi(h,k,l)\,. \end{aligned}$$

From this set of phase relationships it can be seen that the transform along l is the same as for a screw diad (as would be expected since applying the 6_1 three times is equivalent to a 2_1). The following set of transposition relations then holds:

$$\begin{aligned} T_l(k,h,z) &= T^*{}_l(h,k,\tfrac{1}{6}-z) \\ T_l(-k,h+k,z) &= T_l(h,k,\tfrac{1}{6}+z) \\ T_l(-h-k,k,z) &= T_l(h,k,\tfrac{1}{3}-z) \\ T_l(-h-k,h,z) &= T_l(h,k,\tfrac{1}{3}+z) \\ T_l(-h,h+k,z) &= T_l(h,k,\tfrac{1}{2}-z) \end{aligned}$$

from which one twelfth of the z axis may be calculated. This is an asymmetric unit for this space group.

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