symmetry of a 3-D sphere, thus: $\infty/m \,\infty\, \infty''$, or $\infty' \,\infty' \,\infty''$. This has as subgroups all the irreducible 4-D point groups, including those isomorphous with 4-D space groups, enumerated by Coxeter (1934, p. 601). No doubt the (unlisted) reducible groups, which may be formed as a product of two or more groups of lower dimension, are also subgroups of $\infty' \,\infty' \,\infty''$. If other dimensional invariances are added, then such products are sufficient to describe the resulting symmetry; a symbol for this kind of symmetry is composed by bracketing those parts of the symbol that refer to one of the multiplying subgroups. For example, if the dimensional invariance is 2, 4, as in plane color groups, there is freedom within a 2-D plane, and also rotationally within the 2-D 'color plane' that is completely perpendicular in 4-D. The symmetry group is a product of the symmetry groups representing two planes, that is, $(\infty m)(\infty m)$. Di-rotation is present, as when you simultaneously rotate $\pi/2$ and change from red to green in Belov & Tarkhova's (1956, p. 10) group '$P4_1$', but is not essential to a description of the symmetry, that is $(\infty m)(\infty m)\infty'' = (\infty m)(\infty m)$.

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# Anisotropic Structure Factor Calculations.*

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A general form of the anisotropic structure factor which is suitable for evaluation in any space group is presented. A simple scheme for specifying the space group symmetry avoids the use of special 'patches'. The suggested form in the case of general and most special positions reduces to a form which permits substantial savings in the time required to form the function arguments and is well adapted to computation of structure factors and derivatives on high speed digital computers.

## Structure factor for general position

As was demonstrated by Levy (1956), the $\beta_{ij}$ in the expression for the anisotropic temperature factor,

$$\exp\left(-\sum_{i=1}^{3}\sum_{j=1}^{3}\beta_{ij}h_i h_j\right),$$

for symmetrically related positions, transform as do the quadratic products of atomic coordinates, while ignoring translational components.

If $\mathbf{x}^{(1)}$ represents the basic point of a set of equivalent atoms and $\mathbf{x}^{(r)}$ represents another point of the set obtained by the symmetry operation, we can write

$$\mathbf{x}^{(r)} = \mathbf{C}^{(r)}\mathbf{x}^{(1)} + \boldsymbol{\tau}^{(r)} \qquad (1)$$

where $\mathbf{C}^{(r)}$ is a $3 \times 3$ matrix and $\boldsymbol{\tau}^{(r)}$ is a $3 \times 1$ matrix representing a translational vector. While ignoring the $\boldsymbol{\tau}^{(r)}$, we can write

$$x_i^{(r)} = \sum_k C_{ik}^{(r)} x_k^{(1)} \qquad (2)$$

and

$$x_i^{(r)} x_j^{(r)} = \sum_k \sum_l C_{ik}^{(r)} x_k^{(1)} x_l^{(1)} C_{jl}^{(r)} \qquad (3)$$

whence

$$\beta_{ij}^{(r)} = \sum_k \sum_l C_{ik}^{(r)} \beta_{kl}^{(1)} C_{jl}^{(r)} . \qquad (4)$$

If we let

$$M_{\mathbf{h}}^{(r)} = \sum_i^3 \sum_j^3 \beta_{ij}^{(r)} h_i h_j \qquad (5)$$

we can substitute (4) into (5) and obtain

$$M_{\mathbf{h}}^{(r)} = \sum_k^3 \sum_l^3 \beta_{kl}^{(1)} \left( \sum_i C_{ik}^{(r)} h_i \right) \left( \sum_j C_{jl}^{(r)} h_j \right) \qquad (6)$$

$$M_{\mathbf{h}}^{(r)} = \sum_i \sum_j \beta_{ij}^{(1)} H_i^{(r)} H_j^{(r)} \qquad (7)$$

where

$$\mathbf{H}^{(r)} = \mathbf{C}^{(r)T} \mathbf{h} . \qquad (8)$$

The superscript $T$ implies the transpose of the matrix $C^{(r)}$.

The exponent of the geometrical structure factor can be written as

$$\mathbf{h}^T \mathbf{x}^{(r)} = \mathbf{H}^{(r)T} \mathbf{x}^{(1)} + \mathbf{h}^T \boldsymbol{\tau}^{(r)} . \qquad (9)$$

The structure factor for a general set of positions can now be expressed as

$$f \sum_r \exp \left( -\mathbf{H}^{(r)T} \boldsymbol{\beta}^{(1)} \mathbf{H}^{(r)} + 2\pi i (\mathbf{H}^{(r)T} \mathbf{x}^{(1)} + \mathbf{h}^T \boldsymbol{\tau}^{(r)}) \right) . \qquad (10)$$

A center of symmetry or cell centering can be treated in the usual way by using multiplicity factors and summing over the appropriate points of the set. The structure factor in essentially this form is used by Busing & Levy (1959) in their least-squares program.

## Structure factor for special positions

If a set of special positions have symmetry represented by a diagonal matrix, some of the various parameters will be zero or constant and the summation should be carried out either over the points of the special set or over the points of a general set using a multiplicity factor.

If a set of special positions have symmetry represented by a non-diagonal matrix, the situation is somewhat different in that some parameters may be

expressed in linear combinations of the other parameters. One simple way to treat this situation is to consider the 'quadratic' quantities as column vectors such as

$$\begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \\ \beta_6 \end{bmatrix} = \begin{bmatrix} \beta_{11} \\ \beta_{22} \\ \beta_{33} \\ 2\beta_{12} \\ 2\beta_{13} \\ 2\beta_{23} \end{bmatrix} = \begin{bmatrix} Q_{11} \dots Q_{1n} \\ Q_{21} \dots Q_{2n} \\ Q_{31} \dots Q_{3n} \\ Q_{41} \dots Q_{4n} \\ Q_{51} \dots Q_{5n} \\ Q_{61} \dots Q_{6n} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ . \\ . \\ b_n \end{bmatrix} , \qquad (11)$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} P_{11} \dots P_{1m} \\ P_{21} \dots P_{2m} \\ P_{31} \dots P_{3m} \end{bmatrix} \begin{bmatrix} a_1 \\ . \\ a_m \end{bmatrix} , \qquad (12)$$

$$\begin{bmatrix} \mathscr{H}_1 \\ \mathscr{H}_2 \\ \mathscr{H}_3 \\ \mathscr{H}_4 \\ \mathscr{H}_5 \\ \mathscr{H}_6 \end{bmatrix} \begin{bmatrix} H_1 H_1 \\ H_2 H_2 \\ H_3 H_3 \\ H_1 H_2 \\ H_1 H_3 \\ H_2 H_3 \end{bmatrix} . \qquad (13)$$

The $b_i$ are the particular linearly independent set chosen to represent the $\beta_{ij}$. The $\beta_{ij}^{(r)}$ are generated by the use of $\mathbf{Q}$ and the specified $\mathbf{b}$. The $a_i$ are similarly chosen to represent the positional parameters. Since some positional parameters may be constant and not zero, a constant $a_m$ may be required although it is not to be varied. For each kind of 'non-diagonal' special position, the matrices $\mathbf{P}$ and $\mathbf{Q}$ must be supplied. The set is described in terms of the $\mathbf{b}$ and $\mathbf{a}$ vectors. The structure factor now becomes, in a completely general form,

$$f \sum_r \exp \left\{ -\mathbf{b}^T \mathbf{Q}^T \boldsymbol{\mathscr{H}}^{(r)} + 2\pi i (\mathbf{H}^{(r)T} \mathbf{P} \mathbf{a} + \mathbf{h}^T \boldsymbol{\tau}^{(r)}) \right\} . \qquad (14)$$

## Method of calculation

Because of the group properties, we can write

$$\mathbf{C}^{(r)} = \mathbf{N}^{(p)} \mathbf{D}^{(q)} \qquad (15)$$

where the pair $(p)$, $(q)$ have a 1 to 1 correspondence to $(r)$. $D^{(q)}$ are diagonal matrices and the $N^{(p)}$ are non-diagonal matrices in addition to the unit matrix. If we let the pair $s$, $t$ have a 1 to 1 correspondence to $i$, we can write

$$\mathscr{H}_i^{(r)} = \left( \sum_k D_{ss}^{(q)} N_{ks}^{(p)} h_k \right) \left( \sum_k D_{tt}^{(q)} N_{kt}^{(p)} h_k \right)$$
$$= H_s^{(r)} H_t^{(r)} . \qquad (16)$$

The structure factor now becomes

$$f \sum_p \sum_q \exp \left\{ \sum_{\substack{i \\ (s,t)}} D_{ss}^{(q)} D_{tt}^{(q)} \sum_j \left( \sum_k N_{ks}^{(p)} h_k \right) \right.$$

$$\times \left( \sum_k N_{kt}^{(p)} h_k \right) Q_{ij} b_j + 2\pi i \left( \sum_i D_{ii}^{(q)} \sum_j \left( \sum_k N_{ki}^{(p)} h_k \right) P_{ij} a_j \right.$$

$$\left. + \sum_i h_i \tau_i^{(r)} \right) \Big\} . \qquad (17)$$

The structure factor in this form (17) is applicable to any position of any space group. It is easily seen that the presence of the $P_{ij}$ and $Q_{ij}$ terms although required for the evaluation of derivatives complicates the calculation procedure. It would appear therefore, that it would be worthwhile to use form (17) for special positions of 'non-diagonal symmetry' and to investigate the simpler form resulting in diagonal **P** and **Q**. This simpler form is applicable to special positions of 'diagonal symmetry' or to general positions, obtained by setting **P** = **Q** = **1** and is given by

$$f \sum_p \sum_q \exp \left\{ \sum_i D_{ss}^{(q)} D_{tt}^{(q)} \left( \sum_k N_{ks}^{(p)} h_k \right) \left( \sum_k N_{kt}^{(p)} h_k \right) b_i \right.$$
$$\left. + 2\pi i \left( \sum_i D_{ii}^{(q)} \left( \sum_k N_{ki}^{(p)} h_k \right) a_i + \sum_i h_i \tau_i^{(r)} \right) \right\} . \quad (18)$$

If the quantities

$$\left( \sum_i h_i \tau_i^{(r)} \right), \quad \left( \sum_k N_{ki}^{(p)} h_k \right) \quad \text{and} \quad \left( \sum_k N_{ks}^{(p)} h_k \right) \left( \sum_k N_{kt}^{(p)} h_k \right)$$

are formed when the indices $h_i$ are first obtained, no great amount of time is lost. As each set of $b_i$ or $a_i$ are called from storage for calculation, the multiplication by the appropriate

$$\left( \sum_k N_{ki}^{(p)} h_k \right) \quad \text{or} \quad \left( \sum_k N_{ks}^{(p)} h_k \right) \left( \sum_k N_{kt}^{(p)} h_k \right)$$

can be carried out. The subsequent summation over $q$ now has an invariant form, no matter what the value of $p$ may be. This form requires that the arguments of the exponential be obtained as sums or differences of the quantities above, since $D_{ss}^{(q)} D_{tt}^{(q)} = \pm 1$. If the sum of the terms is prepared when the products are formed, each successive argument for a new value of $q$ can be obtained (in a binary computer) by a left shift 1 place of the terms which change sign and subtraction of the results from the sum. A similar procedure will work for the positional parameters. A suitable set of $D^{(q)}$ would be

$$\begin{bmatrix} 100 \\ 010 \\ 001 \end{bmatrix} \quad \begin{bmatrix} 100 \\ 010 \\ 00\bar{1} \end{bmatrix} \quad \begin{bmatrix} 100 \\ 0\bar{1}0 \\ 001 \end{bmatrix} \quad \begin{bmatrix} \bar{1}00 \\ 010 \\ 001 \end{bmatrix} .$$

Each set of position coordinates would specify which of the $(r)$ points should be used in the structure factor sum. As an example, the argument for the thermal factor for the second matrix above would be formed by

$$\sum_i \sum_j h_i h_j \beta_{ij} - 2(2h_1 h_3 \varrho_{13} + 2h_2 h_3 \beta_{23})$$

or in the alternative notation

$$\sum_i \mathscr{H}_i b_i - 2 (\mathscr{H}_5 b_5 + \mathscr{H}_6 b_6) .$$

The proper choice of signs and terms is invariant and can be built into the summation over $q$ part of the program. The summation over $p$ is accomplished by looping and supplying a new set of

$$\left( \sum_k N_{ki}^{(p+1)} h_k \right)$$

and of the products. This procedure results in a substantial saving of multiplication time in the formation of arguments and permits a straight forward treatment of symmetry transformations. In the worst case of 'non-diagonal' special positions, the general routine is used but the specification of the special symmetry is easily made by means of the **P** and **Q**. This avoids the difficulties of writing special patches.

The general form (17) can be handled in the same way, if derivatives are not wanted, by simply entering explicitly without **P** and **Q** each $a_i$ and $b_i$ and either using a multiplicity factor or a selection device to select a desired set of terms. However, if derivatives are desired, the **P** and **Q** matrices are required to form the proper linear combinations.

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