Acta Cryst. (1977). A**33**, 62–70

The Molecular Replacement Method. II. The Translation Function Problem; a New Translation Function

BY D. B. LITVIN

Department of Physics, University of British Columbia, Vancouver, B.C., V6T 1W5, Canada

(*Received 6 December* 1975; *accepted* 24 *August* 1976)

A new translation function, a generalization of the translation function introduced by Rossmann, Blow, Harding, and Coller, is defined. Peaks of this new translation function are related to the orientation and point group of and translation vectors between molecules in a crystal. A method is formulated to determine all peaks of this new translation function corresponding to a given crystal. The applicability of this method is shown in the analysis of translation function data to determine the translation vectors between molecules, and to determine the point group of the molecules when the solution of the rotation function problem is not unique. This new translation function has an advantage over the translation function introduced by Rossmann and co-workers, in that it may contain peaks which are not streaked. It is proposed that this new translation function be used in the structure determination of bovine liver catalase. For trigonal crystalline bovine liver catalase it is shown how this new translation function can be used to determine the point group of and the translation vectors between the catalase molecules.

To determine the structure of biological macromolecules from crystal X-ray diffraction data, without the use of isomorphous derivatives, the 'molecular replacement method' has been developed (Rossmann, 1972). This method consists of three steps:

1. The rotation problem: determining the orientation and point group of the molecules in the crystal.
2. The translation problem: determining the translation vectors between molecules in the crystal.
3. The phase problem: using the information obtained in the first two steps in determining the structure factors.

The methods used in solving the rotation problem are based on the comparison of Patterson functions in different orientations. The Patterson function of the crystal of unknown structure is compared with a Patterson function constructed on the basis of partial knowledge of the molecule's structure (Tollin & Cochran, 1964; Nordman, 1966), with the Patterson function of a known molecule of similar structure (Adams *et al.*, 1970), or when none of the structure is known, with itself (*e.g.* Johnson, Argos, Rossmann & Wagner, 1975). This comparison can be carried out by using the rotation function $\mathscr{R}(A)$ defined by Rossmann & Blow (1962):

$$\mathscr{R}(A)=\int_U P(\mathbf{u})P(A\mathbf{u})\mathrm{d}\mathbf{u} \tag{1}$$

where A is a proper rotation, and the integration is over a volume U dependent on the size and shape of the molecules.

In the case where the Patterson function of the crystal of unknown structure is compared with itself, a method to determine the orientation and point group of the molecules from the peaks of the rotation function, equation (1), has been formulated by Litvin (1975). This formulism has been used in the analysis of the rotation function of crystalline satellite tobacco necrosis virus (STNV) and crystalline bovine liver catalase (Litvin, 1975). As shown in the case of crystalline bovine liver catalase, the solution of the rotation function problem may not be unique (Eventoff & Gurskaya, 1975; Litvin, 1975). Similar methods for solving the translation problem have been used when all or part of the molecule's structure is known (Tollin, 1966; Crowther & Blow, 1967; Huber, 1969), with the use of known molecules of similar structure (Tollin, 1969; Lattman & Love, 1970), and when none of the molecule's structure is known (Rossmann, Blow, Harding & Coller, 1964; Dodson, Harding, Hodgkin & Rossmann, 1966).

In this paper we shall discuss the translation problem, restricting ourselves to the case where none of the molecule's structure is known. The method which has been used to determine the translation vectors, in this case, is based on the analysis of peaks of the translation function $T(\mathbf{x})$ introduced by Rossmann *et al.* (1964).

$$T(\mathbf{x})=\int_U P(\mathbf{x}+\mathbf{u})P(-\mathbf{x}+C_2\mathbf{u})\mathrm{d}\mathbf{u}$$

where $P(\mathbf{r})$ denotes the Patterson function of the unknown crystal, C_2 a rotation of 180°, and where, as in the rotation function, equation (1), the volume U is dependent on the size and shape of the molecules.

Using the inversion symmetry property of the Patterson function, we will rewrite and denote this translation function as

$$T(\mathbf{x},m)=\int_U P(\mathbf{x}+\mathbf{u})P(\mathbf{x}+m\mathbf{u})\mathrm{d}\mathbf{u} \tag{2}$$

where $m=\bar{C}_2$ is a mirror plane, the product of inversion $\bar{1}$ and the rotation C_2. We have denoted this translation function as $T(\mathbf{x},m)$ to denote explicity the mirror plane m appearing on the right-hand side. As has been pointed out (Rossmann *et al.*, 1964; Rossmann, 1973), from this translation function, for a specific mirror plane, one can determine only the components of the peaks, and consequently of the translation vectors, perpendicular to this mirror plane. Only by using three different mirror planes, *i.e.* three different orientations of the mirror plane m, is there the possibility of uniquely determining the translation vectors. In addition, there is no general formulism available which relates the point group and orientation of and translation vectors between molecules of the crystal with the positions of the peaks of this translation function.

It is the purpose of this paper to introduce and determine the properties of a new translation function which is a generalization of the translation function given above. This new translation function is

$$T(\mathbf{x},A)=\int_U P(\mathbf{x}+\mathbf{u})P(\mathbf{x}+A\mathbf{u})\mathrm{d}\mathbf{u} \qquad (3)$$

where A is an arbitrary rotation, and where the integration is over the same volume U as in equation (2).* In the special case when $A=m$, this new translation function becomes identical with equation (2), with the translation function given by Rossmann *et al.* (1964). When $\mathbf{x}=0$ and A is a proper rotation, equation (3) is identical with equation (1), the rotation function given by Rossmann & Blow (1962).

In the following section a method is formulated to determine the values of $\mathbf{x}$ and A corresponding to all peaks of the translation function $T(\mathbf{x},A)$ by determining the relationship between these values of $\mathbf{x}$ and A, the point group and orientation of and translation vectors between the molecules in the crystal. We shall also determine the behaviour of $T(\mathbf{x},A)$ in the neighborhood of its peaks and consequently show that from a translation function $T(\mathbf{x},A)$ for one specific value of A, when $A=\bar{C}_N$, $N\neq 2$, an N-fold rotation–inversion, one can determine all components of the peaks.

In the final section we consider the case of trigonal crystalline bovine liver catalase. Using the formulism of the previous section, we determine the dependence of the positions of the peaks of the translation function $T(\mathbf{x},\bar{C}_4)$, for a specific fourfold rotation–inversion, on the point group and orientation of and translation vectors between the bovine liver catalase molecules. It is then shown how one can determine the positions of the molecules from the positions of the peaks of this translation function. In addition, it is shown that this translation function can be used as a 'test function' to determine uniquely which of the two solutions of the rotation problem is the point group of the bovine liver catalase molecules.

The translation function $T(\mathbf{x},A)$

As the translation function $T(\mathbf{x},A)$, equation (3), is defined in terms of the Patterson function, we begin by reviewing some properties of the Patterson function: The Patterson function of a crystal made up of molecules can be written in the form

$$P(\mathbf{r})=\sum_{jkt} P_{jkt}(\mathbf{r}) \qquad (4)$$

where j and k index the molecules in the unit cell, and t the translations of the space group of the crystal. $P_{jj0}(\mathbf{r})$ represents the contribution to the Patterson function of the 'self-vectors' (intramolecular vectors or self-Patterson) of the jth molecule, and $P_{jkt}(\mathbf{r})$, the 'cross-vectors' (intermolecular vectors or cross-Patterson) between the jth molecule in the first unit cell and the kth molecule in the tth unit cell.

We will denote by $\mathbf{\Delta}_{jk}$ the translation vector between the positions of the jth and kth molecule in the unit cell. Substituting $\mathbf{r}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{u}$ we can rewrite the contribution of the (jkt)th cross-vectors as $P_{jkt}(\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{u})$ which we then interpret as a function of the vector variable $\mathbf{u}$ whose origin is at $\mathbf{r}=\mathbf{\Delta}_{jk}+\mathbf{t}$. We will say that the (jkt)th cross-vectors are centred at $\mathbf{r}=\mathbf{\Delta}_{jk}+\mathbf{t}$ and, since the molecules are of finite dimension, localized within a volume U about $\mathbf{r}=\mathbf{\Delta}_{jk}+\mathbf{t}$. The Patterson function can thus be considered as a superposition of overlapping arrays of self-vectors and cross-vectors centred at positions $\mathbf{r}=\mathbf{\Delta}_{jk}+\mathbf{t}$.

The translation function $T(\mathbf{x},A)$, equation (3), is an overlap integral of a volume U of the Patterson centred at $\mathbf{x}$, *i.e.* $P(\mathbf{x}+\mathbf{u})$ where $\mathbf{u}$ is restricted to be within the volume U, and a rotated image of this same volume. The translation function $T(\mathbf{x},A)$ is non-zero if all or part of this volume is identical with its rotated image. This volume of the Patterson function may intersect one or more of the arrays of cross-vectors. Therefore, the non-zero values of the $T(\mathbf{x},A)$ are associated with either the transformation of one array of cross-vectors into itself, or into a second array of cross-vectors. Relative maxima of the translation function $T(\mathbf{x},A)$ considered as a function of $\mathbf{x}$, for constant A, will be called 'peaks' of the translation function. Peaks then

---

* Electron microscopy is helpful in determining the volume U in the case of 'spherical viruses', *e.g.* satellite tobacco necrosis virus (STNV) (Fridborg *et al.*, 1965). The effect of the choice of the volume U on the resolution of rotation function peaks, in the case of STNV, has been discussed by Lentz & Strandberg (1974).

In the third step of the molecular replacement method, the phase problem, not discussed in this paper, the related problem of determining the volume to be used in real space averaging of the electron density (Bricogne, 1974; Argos, Ford & Rossmann, 1975) has been named the 'Molecular Envelope Problem' (Bricogne, 1976). The choice of this volume, in the phasing of lobster GPD, as a sphere, has been shown to be inadequate (Argos *et al.*, 1975).

The purpose of this paper is to discuss not the phase problem but the translation problem, and introduce the new translation function, equation (3), which is a generalization of equations (1) and (2). As the same volume is used in both translation functions, equations (2) and (3), and as the usefulness of Rossmann & Blow's (1962) rotation function, equation (1), and Rossmann *et al.*'s (1964) translation function, equation (2), has been shown, in spite of the problem of choosing the volume U, we shall assume that the volume U has somehow been defined.

correspond to the case where all or part of a volume U of the Patterson function is identical with its rotated image and where, at the same time, its intersection with an array or arrays of cross-vectors, as a function of $\mathbf{x}$, is maximum.

We shall now determine the relationship between the values of $\mathbf{x}$ and A corresponding to all peaks of the translation function $T(\mathbf{x},A)$ and the point group and orientation of and translation vectors between molecules in the crystal: Consider all pairs of arrays of cross-vectors $P_{jkt}(\mathbf{r})$ and $P_{j'k't'}(\mathbf{r})$. Necessary and sufficient conditions that the translation function $T(\mathbf{x},A)$ has non-zero values associated with the transformation of $P_{jkt}(\mathbf{r})$ into $P_{j'k't'}(\mathbf{r})$ are as follows:

(1) the rotation A is such that

$$P_{jkt}(\boldsymbol{\Delta}_{jk}+\mathbf{t}+A^{-1}\mathbf{u})=P_{j'k't'}(\boldsymbol{\Delta}_{j'k'}+\mathbf{t}'+\mathbf{u}), \tag{5}$$

that is, the array of cross-vectors $P_{j'k't'}(\mathbf{r})$ is identical with the array of cross-vectors $P_{jkt}(\mathbf{r})$ after the latter has been rotated about its centre, at $r=\boldsymbol{\Delta}_{jk}+\mathbf{t}$, by the rotation A.

(2) The rotation A and position $\mathbf{x}$ are such that

$$A(\boldsymbol{\Delta}_{jk}+\mathbf{t}-\mathbf{x})=\boldsymbol{\Delta}_{j'k'}+\mathbf{t}'-\mathbf{x}, \tag{6}$$

that is, under the rotation A about $\mathbf{x}$, the centre of the array of cross-vectors $P_{jkt}(\mathbf{r})$ is transformed into the centre of the array of cross-vectors $P_{j'k't'}(\mathbf{r})$.

(3) The vector $\frac{1}{2}\mathbf{y}$, where $\mathbf{y}=\boldsymbol{\Delta}_{jk}+\mathbf{t}-\mathbf{x}$ is within the volume U.

The first two of these conditions demand that the array of cross-vectors $P_{jkt}(\mathbf{r})$ is transformed by the rotation A about $\mathbf{x}$ into the array of cross-vectors $P_{j'k't'}(\mathbf{r})$, the third condition, that the volume U of the Patterson function centred at $\mathbf{x}$ intersects both arrays of cross-vectors.

In determining the peaks of the translation function from the above conditions, we limit ourselves to the case where the molecular positions in the first unit cell are general positions and constitute one set of equivalent positions with respect to the space group of the crystal. The general case is discussed in Appendix I.

Let R_i denote a rotation of the space group of the crystal, and $\mathbf{P}$ the point group of the molecule at position $\mathbf{r}_1$ in the unit cell. The position $\mathbf{r}_i$ of the ith molecule in the unit cell is then given by $\mathbf{r}_i=R_i\mathbf{r}_1+\boldsymbol{\tau}(R_i)$, where $\boldsymbol{\tau}(R_i)$ is the non-primitive translation associated with R_i. We denote by $\{R(jk)\}$ the set of all rotations which rotate the molecule at $\mathbf{r}_j$ into the orientation of the molecule at $\mathbf{r}_k$. It has been shown (Litvin, 1975) that:

$$\{R(jk)\}=\{R_k\mathbf{P}R_j^{-1}\} \tag{7}$$

where $\{R_k\mathbf{P}R_j^{-1}\}$ denotes the set of all rotations of the form $R_kPR_j^{-1}$ where P is an element of $\mathbf{P}$.

A set of rotations which satisfies the first condition, equation (5), for two arrays of cross-vectors $P_{jkt}(\mathbf{r})$ and $P_{j'k't'}(\mathbf{r})$ will be denoted by

$$\{A(jkj'k')\}=[\{R(jj')\}\cap\{R(kk')\}] + \bar{1}[\{R(jk')\}\cap\{R(kj')\}] \tag{8}$$

where the symbol $\cap$ means 'intersection', *i.e.* $\{R(jj')\}\cap\{R(kk')\}$ means 'those rotations contained in *both* the sets of rotations $\{R(jj')\}$ and $\{R(kk')\}$'.

We shall assume that there are no other rotations which satisfy this condition.* If the set of rotations $\{A(jkj'k')\}$ is empty, then the two arrays of cross-vectors $P_{jkt}(\mathbf{r})$ and $P_{j'k't'}(\mathbf{r})$ are not congruent.

If A is a rotation contained in $\{A(jkj'k')\}$ then the translation function $T(\mathbf{x},A)$ will be non-zero for those values $\mathbf{x}$ which satisfy the second condition, equation (6). The value of $\mathbf{x}$ is given by

$$\mathbf{x}=\boldsymbol{\Delta}_{jk}+\mathbf{t}+\mathbf{y} \tag{9}$$

where the vector $\mathbf{y}$ must satisfy the equation:

$$\mathbf{y}-A\mathbf{y}=\boldsymbol{\Delta}_{j'k'}-\boldsymbol{\Delta}_{jk}+\mathbf{t}'-\mathbf{t}. \tag{10}$$

If there is no solution to equation (10), or if the vector $\mathbf{y}$ does not satisfy the third condition, then the translation function $T(\mathbf{x},A)$ for this rotation A, will be zero.

We distinguish between three cases with respect to the rotation A:

(1) $A=C_N$: If A is a N-fold proper rotation, $N\neq 1$, a solution of equation (10) exists if and only if the component of the vector $\boldsymbol{\Delta}_{j'k'}-\boldsymbol{\Delta}_{jk}+\mathbf{t}'-\mathbf{t}$ parallel to the rotation axis of C_N is zero. If so, then the translation function $T(\mathbf{x},C_N)$ is non-zero for $\mathbf{x}=\boldsymbol{\Delta}_{jk}+\mathbf{t}+\mathbf{y}_\perp+\mathbf{y}_\parallel$ where $\mathbf{y}_\perp$ is the vector perpendicular to the rotation axis of C_N which is determined from equation (10), and $\mathbf{y}_\parallel$ is an arbitrary vector parallel to the rotation axis of C_N. Because of the arbitrariness of $\mathbf{y}_\parallel$, limited of course by condition (3), the translation function $T(\mathbf{x},C_N)$ will be non-zero for those values of $\mathbf{x}$ along a line passing through the point $\mathbf{x}=\boldsymbol{\Delta}_{jk}+\mathbf{t}+\mathbf{y}_\perp$ and parallel to the rotation axis of C_N.

The maximum value of the translation function $T(\mathbf{x},C_N)$ along this line of non-zero values is at $\mathbf{x}=\boldsymbol{\Delta}_{jk}+t+\mathbf{y}_\perp$, *i.e.* when $\mathbf{y}_\parallel=0$. To exemplify this, consider the case where both the arrays of cross-vectors are taken as $P_{jk0}(\mathbf{r})$ and assume that $\{A(jkjk)\}$ contains the proper rotation C_N, $N\neq 1$, *i.e.* $P_{jk0}(\mathbf{r})$ is invariant under the rotation C_N about its centre at $\mathbf{r}=\boldsymbol{\Delta}_{jk}$. In this case equation (10) becomes $\mathbf{y}-C_N\mathbf{y}=0$ and consequently $\mathbf{y}_\perp=0$. The translation function is therefore non-zero for $\mathbf{x}=\boldsymbol{\Delta}_{jk}+\mathbf{y}_\parallel$, see equation (9), where $\mathbf{y}_\parallel$ is an arbitrary vector. When $\mathbf{y}_\parallel=0$ the centre of the volume U of the Patterson is centred at $\mathbf{x}=\boldsymbol{\Delta}_{jk}$ and the inter-

---

* It is easily shown that rotations contained in equation (8) satisfy equation (5), and we have assumed that there are no additional rotations with this property. Such an assumption is basic to this analysis of the translation function and no justification will be given other than to point out similar assumptions which have been implicitly used in the analysis of the translation function $T(\mathbf{x},m)$ (Rossmann *et al.*, 1964) and of the rotation function (Litvin, 1975). In the former, using the notation of this paper, it was shown that $T(\mathbf{x},m)$ contains a peak if for some j and k, $\{A(jkjk)\}$ contains an element $A=m$; it was implicitly assumed that $T(\mathbf{x},m)$ contains no other peaks. In the latter, it was stated that if $\mathbf{P}$ is the symmetry point group of a molecule, then the symmetry point group of the corresponding array of self-vectors is $\mathbf{P}\times\bar{1}$. That $\mathbf{P}\times\bar{1}$ is an invariance group of the array of self-vectors is easily shown; that $\mathbf{P}\times\bar{1}$ is the symmetry group was assumed.

section of this volume and the array of cross-vectors $P_{jk0}(\mathbf{r})$, also centred at $\mathbf{x}=\mathbf{\Delta}_{jk}$, is maximum. Therefore the translation function $T(\mathbf{x},C_N)$ has a peak at $\mathbf{x}=\mathbf{\Delta}_{jk}$, when $\mathbf{y}_{\|}=0$, and decreases in value when $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{y}_{\|}$ as the intersection of the volume U of the Patterson and the array of cross-vectors $P_{jk0}(\mathbf{r})$ decreases.

Consequently, in general, there is a peak of the translation function $T(\mathbf{x},C_N)$ at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}_{\perp}$ and in addition the translation function is non-zero for those values of $\mathbf{x}$ along a line passing through the peak and parallel to the rotation axis of C_N. We shall say that $T(\mathbf{x},C_N)$ has a peak at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}_{\perp}$ and 'streaking' of this peak in the direction of the rotation axis of C_N.

(2) $A=m$: This is the case of the translation function, equation (1), used by Rossmann *et al.* (1964). If A is a mirror plane, a solution of (10) exists if and only if the component of the vector $\mathbf{\Delta}_{j'k'}-\mathbf{\Delta}_{jk}+\mathbf{t}'-\mathbf{t}$ parallel to the reflexion plane is zero. If so, then the translation function $T(\mathbf{x},m)$ is non-zero for $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}_{\perp}+\mathbf{y}_{\|}$ where $\mathbf{y}_{\perp}$, a vector perpendicular to the mirror plane, is determined from equation (10), and $\mathbf{y}_{\|}$ is an arbitrary vector parallel to the mirror plane m. The translation function $T(\mathbf{x},m)$ has a peak at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}_{\perp}$, *i.e.* when $\mathbf{y}_{\|}=0$, and is non-zero for values of $\mathbf{x}$ on a plane passing through this peak and parallel to the reflexion plane m. We shall say that there is a peak of the translation function $T(\mathbf{x},m)$ at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}_{\perp}$ and 'smearing' of this peak in a plane parallel to m.* It is the smearing of the peaks which, as pointed out by Rossmann (1973), makes it possible in practice only to determine the component of the peaks $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}_{\perp}$ in the direction perpendicular to the reflexion plane $m=\bar{C}_2$, *i.e.* parallel to the axis of the twofold rotation C_2.

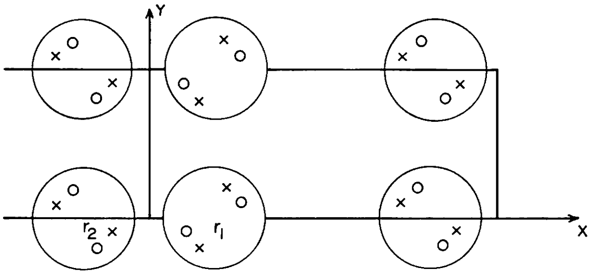

Fig. 1. Model of crystal of space group $P121$ (C_2^1) with two molecules in the unit cell. The point group of the molecule at the general position $\mathbf{r}_1=(x,0,z)$ is $2_{xy}2_{xy}2_z$ $[D_2^{(xy,\bar{x}y,z)}]$. Only four atoms of each molecule are shown explicitly, and only the molecules whose Z component is $\pm z$ are depicted. Atoms of a molecule lying above and below a plane parallel to the crystallographic XY plane and passing through the molecule's centre are denoted by ○ and × respectively.

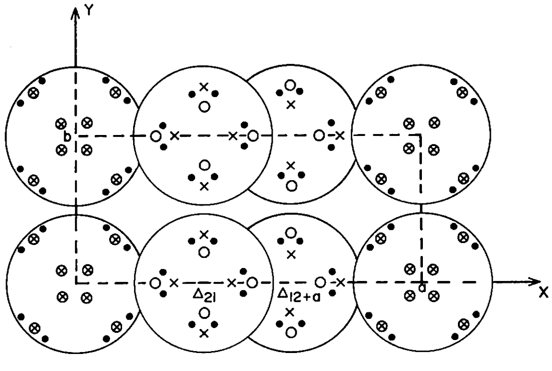

Fig. 2. Patterson function of the model crystal given in Fig. 1. Only the arrays of self-vectors and cross-vectors related to the molecules depicted in Fig. 1 are shown. The self-vectors and cross-vectors related to the atoms explicitly shown in Fig. 1, above, on, and below planes parallel to the crystallographic XY plane and passing through the centres of the arrays of self-vectors and cross-vectors, are denoted by ○, ●, and ×, respectively. The centres of the arrays are also indicated.

(3) $A=\bar{C}_N$, $N\neq 2$: If A is an N-fold rotation–inversion, with $N\neq 2$, then the translation function $T(\mathbf{x},\bar{C}_N)$ is non-zero for $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}$, where $\mathbf{y}$ is uniquely determined from equation (10). In this case, $T(\mathbf{x},\bar{C}_N)$ is non-zero at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}$, and, because of the uniqueness of the solution of equation (10), zero in the neighbourhood of this point. Consequently $T(\mathbf{x},\bar{C}_N)$ has a peak at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}+\mathbf{y}$ and there is no streaking nor smearing of the peak.

The strongest peaks of the translation function $T(\mathbf{x},A)$ correspond to the case where $j=j'$ and $k=k'$, for rotations A in $\{A(jkjk)\}$, and are at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}$. This follows from the fact that at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}$ the volume U coincides with the array of cross-vectors $P_{jkt}(\mathbf{r})$, and that these rotations leave the array of cross-vectors $P_{jkt}(\mathbf{r})$ invariant. We shall refer to these peaks at $\mathbf{x}=\mathbf{\Delta}_{jk}+\mathbf{t}$ as the *dominating peaks* of the translation function.

By using equations (8), (9), and (10), for all possible values of the indices j, k, j', and k' one determines the position of all peaks of the translation function $T(\mathbf{x},A)$, and the relationship between the positions of these peaks and the point group and orientation of and translation vectors between molecules in the crystal. By comparing the positions of peaks of the translation function $T(\mathbf{x},A)$ predicted by the above method with the positions of peaks of $T(\mathbf{x},A)$ calculated from experimental data, one can obtain information on the translation vectors. However, in determining the positions of the peaks, problems arise in the cases where $A=C_N$ and m, the latter corresponding to the translation function used by Rossmann *et al.* (1964), because of the streaking or smearing of the peaks. An advantage of the translation function introduced in this paper over the one used by Rossmann *et al.* (1964), is that if there are peaks of the translation function $T(\mathbf{x},\bar{C}_N)$, $N\neq 2$, these peaks are neither streaked nor smeared.

---

* The term 'streaking', instead of 'smearing', has been used to describe the behaviour of the translation function $T(\mathbf{x},m)$ in the neighborhood of its peaks (*e.g.* Blow, Rossmann & Jeffers, 1964). However, this author believes that the term 'smearing' more adequately describes the two-dimensional arbitrariness of the solutions of equation (10) in this case where $A=m$, and reserves the term 'streaking' for the case where $A=C_N$, $N\neq 1$, where there is a one-dimensional arbitrariness of the solutions of equation (10).

Finally, we would like to point out that in the paper by Rossmann *et al.* (1964) where the translation function $T(\mathbf{x},m)$, equation (2), was introduced, the translation function $T(\mathbf{x},A)$, equation (3), was implicitly considered, but rejected. The rejection of $T(\mathbf{x},A)$ was due to the lack of a general method, as the one presented in this paper, to predict all peaks of a translation function. The reasoning which lend to their erroneous rejection of the translation function $T(\mathbf{x},A)$, is considered in Appendix II.

As a simple example of the above, which shows the advantages of using this new translation function, consider a crystal of the space group $P121$ (C_2^1) with two molecules in the unit cell. In a Cartesian coordinate system this space group is generated by $(1|a,0,0)$, $(1|0,b,0)$, $(1|c,0,e)$, and $(2y|0,0,0)$ where a, b, c, and e are lattice parameters. The positions of the molecules in the unit cell will be taken as the general positions $\mathbf{r}_1=(x,0,z)$ and $\mathbf{r}_2=2_y\mathbf{r}_1=(\bar{x},0,\bar{z})$, and we assume that the point group of the molecule at $\mathbf{r}_1$ is $2_{xy}2_{xy}2_z$ $[D_2^{(xy,\,xy,\,z)}]$ (*n.b.*: 2_{xy} denotes a rotation of 180° about an axis in the $[1,1,0]$ direction). A schematic representation of this crystal is given in Fig. 1, and its Patterson function in Fig. 2. In Fig. 1, we show explicitly only four atoms of each molecule as a pedagogical aid for visualizing the point group and orientation of the molecules. We emphasize that this and the molecular envelope also depicted are visual aids only, and that, as shown above, the positions of the peaks of the translation function depend only on the point group and orientation of and translation vectors between the molecules.

In this example $R_1=1$, $R_2=2_y$, $\mathbf{P}=2_{xy}2_{\bar{x}y}2_z$ $[D_2^{(xy,\,\bar{x}y,\,z)}]$, and the sets of rotations $\{R(jk)\}$ defined by (7) are tabulated in Table 1. The sets of rotations $\{A(jk,j'k')\}$ determined from equation (8) and Table 1, are tabulated in Table 2. Finally, the values of $\mathbf{x}$ and A, where $\mathbf{x}\neq 0$, of peaks of the translation function $T(\mathbf{x},A)$ corresponding to the arrays of cross-vectors of the Patterson function in Fig. 2, are given in Table 3.

From Table 3 one finds that from the peaks of the translation function $T(\mathbf{x},\bar{4}_z)$, because there is neither streaking nor smearing of these peaks, one can determine $\mathbf{\Delta}_{12}$ and $\mathbf{\Delta}_{21}$. Note also, see Fig. 2, that while the arrays of cross-vectors do overlap, this overlapping will not affect the positions of the peaks. One can also determine, for example, $\mathbf{\Delta}_{12}$ from any two of the translation functions $T(\mathbf{x},2_z)$, $T(\mathbf{x},2_{xy})$ and $T(\mathbf{x},2_{\bar{x}y})$ since each of these has a peak which is streaked at $\mathbf{x}=\mathbf{\Delta}_{jk}$.

Table 1. *The sets of rotations* $\{R(jk)\}=\{R_kPR_j^{-1}\}$, $j,k=1,2$, *tabulated for* $\mathbf{P}=2_{xy}2_{\bar{x}y}2_z$ $[D_2^{(xy,\,\bar{x}y,\,z)}]$ *and* $R_1=1$ *and* $R_2=2_y$

j	k	$\{R(jk)\}$			
1	1	E	2_{xy}	$2_{\bar{x}y}$	2_z
1	2	2_x	2_y	4_z	4_z^3
2	1	2_x	2_y	4_z	4_z^3
2	2	E	2_{xy}	2_{xy}	2_z

Table 2. *The sets of rotations*

$$\{A(jk,j'k')\}=[\{R(jj')\}\cap\{R(kk')\}]+\bar{1}[\{R(jk')\}\cap\{R(kj')\}]$$

for $j,k,j',k'=1,2$

The sets of rotations $\{R(jk)\}$ are given in Table 1.

jk	$j'k'$	$[A(jk,j'k')]=[\{R(jj')\}\cap\{R(kk')\}]+\bar{1}[\{R(jk')\}\cap\{R(kj')\}]$							
11	11	1	$2_{\bar{x}y}$	2_{xy}	2_z	m_{xy}	$m_{\bar{x}y}$	m_z	$\bar{1}$
11	12								
11	21								
11	22	2_x	2_y	4_z	4_z^3	m_x	m_y	$\bar{4}_z$	$\bar{4}_z^3$
12	11								
12	12	1	$2_{\bar{x}y}$	2_{xy}	2_z	m_x	m_y	$\bar{4}_z$	$\bar{4}_z^3$
12	21	2_x	2_y	4_z	4_z^3	m_{xy}	$m_{\bar{x}y}$	m_z	$\bar{1}$
12	22								
21	11								
21	12	2_x	2_y	4_z	4_z^3	m_{xy}	$m_{\bar{x}y}$	m_z	$\bar{1}$
21	21	1	2_{xy}	$2_{\bar{x}y}$	2_z	m_x	m_y	$\bar{4}_z$	$\bar{4}_z^3$
21	22								
22	11	2_x	2_y	4_z	4_z^3	m_x	m_y	$\bar{4}_z$	$\bar{4}_z^3$
22	12								
22	21								
22	22	1	2_{xy}	$2_{\bar{x}y}$	2_z	m_{xy}	$m_{\bar{x}y}$	m_z	$\bar{1}$

Table 3. *Peaks of the translation function* $T(\mathbf{x},A)$ *of the model crystal shown in Fig.* 1 *tabulated according to the rotation A associated with the peak*

A	$\mathbf{x}$
2_z	$\Delta_{21}, \Delta_{21}+\mathbf{t}_x, \frac{1}{2}\mathbf{t}_y, \Delta_{21}+\frac{1}{2}\mathbf{t}_y, \Delta_{12}+\mathbf{t}_x+\frac{1}{2}\mathbf{t}_y$
2_{xy}	$\Delta_{21}, \Delta_{12}+\mathbf{t}_x$
2_{xy}	$\Delta_{21}, \Delta_{12}+\mathbf{t}_x$
2_x	$\frac{1}{2}\mathbf{t}_y$
4_z	$\frac{b}{2}(1,1,0), \frac{b}{2}(-1,1,0)+\mathbf{t}_x$
4_z^3	$\frac{b}{2}(1,1,0), \frac{b}{2}(-1,1,0)+\mathbf{t}_x$
m_x	$\Delta_{21}, \Delta_{12}+\mathbf{t}_x$
m_y	$\Delta_{21}, \Delta_{12}+\mathbf{t}_x, \frac{1}{2}\mathbf{t}_y, \Delta_{21}+\frac{1}{2}\mathbf{t}_y, \Delta_{12}+\mathbf{t}_x+\frac{1}{2}\mathbf{t}_y$
$\bar{1}$	$\frac{1}{2}\mathbf{t}_x, \frac{1}{2}(\mathbf{t}_x+\mathbf{t}_y)$
$\bar{4}_z$	$\Delta_{21}, \Delta_{12}+\mathbf{t}_x, \frac{b}{2}(1,1,0), \frac{b}{2}(-1,1,0)+\mathbf{t}_x$ $\Delta_{21}+\frac{b}{2}(1,1,0), \Delta_{21}+\frac{b}{2}(-1,1,0)$ $\Delta_{12}+\mathbf{t}_x+\frac{b}{2}(1,1,0), \Delta_{12}+\mathbf{t}_x+\frac{b}{2}(-1,1,0)$
$\bar{4}_z^3$	$\Delta_{21}, \Delta_{12}+\mathbf{t}_x, \frac{b}{2}(1,1,0), \frac{b}{2}(-1,1,0)+\mathbf{t}_x$ $\Delta_{21}+\frac{b}{2}(1,1,0), \Delta_{21}+\frac{b}{2}(-1,1,0)$ $\Delta_{12}+\mathbf{t}_x+\frac{b}{2}(1,1,0), \Delta_{12}+\mathbf{t}_x+\frac{b}{2}(-1,1,0)$

By using only the translation function $T(\mathbf{x},m)$ used by Rossmann *et al.* (1964), one cannot uniquely determine the translation vector $\mathbf{\Delta}_{12}$ or $\mathbf{\Delta}_{21}$. From $T(\mathbf{x},m_x)$ and $T(\mathbf{x},m_y)$, because of the smearing of the peaks, one can determine only the x and y components, respectively, of $\mathbf{\Delta}_{12}$ and $\mathbf{\Delta}_{21}$.

Lastly, since in this simple example, $\mathbf{\Delta}_{12}=2\mathbf{r}_1=-2\mathbf{r}_2$, having determined $\mathbf{\Delta}_{12}$, one has also determined the positions of the molecules in the unit cell.

Bovine liver catalase

Trigonal crystalline bovine liver catalase is a crystal with space-group symmetry $P3_121$ (D_3^4) and the positions of the molecules in the unit cell constitute a single set of equivalent positions. X-ray diffraction studies have shown that this catalase molecule has at least one twofold axis of symmetry (Glauser & Rossmann, 1966; Gurskaya, Lubanova & Vainshtein, 1971). Electron microscopy studies indicate that the bovine liver catalase molecule consists of four subunits and has the point group 222 (D_2) (Barynin & Vainshtein, 1971). A rotation function study of trigonal crystalline bovine liver catalase was performed by Eventoff & Gurskaya (1975) and the solution of the rotation function problem (Litvin, 1975) has shown that the point group of the bovine liver catalase molecule is either 4 (C_4) or 222 (D_2).

In this section, using the translation function $T(\mathbf{x},A)$, equation (3), and the method to determine the peaks of this translation function derived in the previous section, we will predict the positions of peaks of a translation function which can be used to determine which of the two point groups is the point group of the bovine liver catalase molecule. We will then show how one can determine, from the positions of these peaks, the positions of the bovine liver catalase molecules in the unit cell of this crystal.

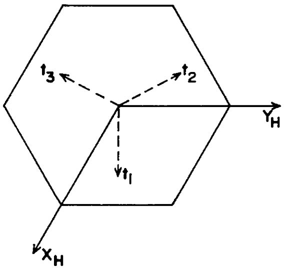

Fig. 3. The orientation of the generators $\mathbf{t}_1,\mathbf{t}_2,\mathbf{t}_3$ of the primitive translations of the trigonal space group $P3_121$ (D_3^4) is shown with respect to the X_H and Y_H axes of the space group's hexagonal unit cell.

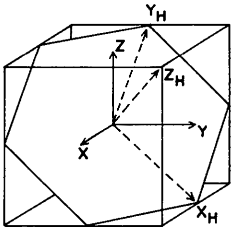

Fig. 4. The hexagonal coordinate system (X_H, Y_H, Z_H) of trigonal crystalline bovine liver catalase is shown relative to the Cartesian coordinate system (X, Y, Z) in which the rotations associated with peaks of the translation function are defined.

In Fig. 3 we show the generators of the primitive translations of the trigonal lattice of $P3_121$ (D_3^4) with respect to a hexagonal coordinate system (X_H, Y_H, Z_H). These generators, denoted by $\mathbf{t}_1$, $\mathbf{t}_2$ and $\mathbf{t}_3$, given in terms of this hexagonal coordinate system are $\mathbf{t}_1=(\frac{2}{3}a,\frac{1}{3}a,\frac{1}{3}c)$, $\mathbf{t}_2=(-\frac{1}{3}a,\frac{1}{3}a,\frac{1}{3}c)$, and $\mathbf{t}_3=(-\frac{1}{3}a,-\frac{2}{3}a,\frac{1}{3}c)$, where a and c are the lattice parameters of the hexagonal unit cell. The positions of the six molecules in the unit cell will be denoted by

$$\begin{array}{ll} \mathbf{r}_1 & \mathbf{r}_4=2_{X_HY_H}\mathbf{r}_1 \\ \mathbf{r}_2=3^2_{Z_H}\mathbf{r}_1+2\boldsymbol{\tau} & \mathbf{r}_5=2_{X_H}\mathbf{r}_1+2\boldsymbol{\tau} \\ \mathbf{r}_3=3_{Z_H}\mathbf{r}_1+\boldsymbol{\tau} & \mathbf{r}_6=2_{Y_H}\mathbf{r}_1+\boldsymbol{\tau} \end{array} \tag{11}$$

where $\boldsymbol{\tau}=(0,0,\frac{1}{3}c)$. The rotations A of the translation function $T(\mathbf{x},A)$ will be given, for simplicity of notation, in a Cartesian coordinate system (X, Y, Z) whose orientation with respect to the above hexagonal coordinate system is shown in Fig. 4.

From the solution of the rotation function problem for trigonal crystalline bovine liver catalase (Litvin, 1975) the point group $\mathbf{P}$ of the molecule at $\mathbf{r}_1$ was determined to be either 4_X [$C_4^{(X)}$] or $2_X2_Y2_Z$ [$D_2^{(X,Y,Z)}$].

In Table 4 we list the sets of rotations $\{A(jk,jk)\}$, $j\neq k, j,k=1,2,\ldots,6$, defined in equation (8), for each of the two point groups. These rotations are associated with the 'dominating' peaks of the translation function $T(\mathbf{x},A)$, where $\mathbf{x}\neq\mathbf{t}$. As seen from Table 4, there are such dominating peaks in, for example, the translation function $T(\mathbf{x},\bar{4}_X)$ in the case where $\mathbf{P}=222$ (D_2) while none in the case where $\mathbf{P}=4$ (C_4). Consequently, we can use the translation function $T(\mathbf{x},\bar{4}_X)$ as a test function to determine which of the two point groups

Table 4. *The sets of rotations $\{A(jk,jk)\}$ tabulated for the models of trigonal crystalline bovine liver catalase for the two cases where the point group of the molecules is* 222 (D_2) *and* 4 (C_4)

jk				$\mathbf{P}=D_2^{(x,y,z)}$				*jk*				$\mathbf{P}=C_4^{(x)}$				
12	1	2_x	2_y	2_z				12	1	$\bar{1}2_{xz}$						
13	1	2_x	2_y	2_z				13	1	$\bar{1}2_{xy}$						
14	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{x}y}$	4_z	4_z^3	$2_{xy}]$	14	1	$\bar{1}2_{\bar{x}y}$						
15	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{y}z}$	2_{yz}	4_x	$4_x^3]$	15	1	4_x	2_x	$4_x^3+\bar{1}[2_y$	2_z	$2_{\bar{y}z}$	$2_{yz}]$	
16	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{x}z}$	2_{xz}	4_y	$4_y^3]$	16	1	$\bar{1}2_{\bar{x}y}$						
23	1	2_x	2_y	2_z				23	1	$\bar{1}2_{yz}$						
24	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{y}z}$	2_{yz}	4_x	$4_x^3]$	24	1	$\bar{1}2_{\bar{y}z}$						
25	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{x}z}$	2_{xz}	4_y	$4_y^3]$	25	1	$\bar{1}2_{\bar{x}z}$						
26	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{x}y}$	2_{xy}	4_z	$4_z^3]$	26	1	4_z	2_z	$4_z^3+\bar{1}[2_x$	2_y	$2_{\bar{x}y}$	$2_{xy}]$	
34	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{x}z}$	2_{xz}	4_y	$4_y^3]$	34	1	4_y	2_y	$4_y^3+\bar{1}[2_x$	2_z	$2_{\bar{x}z}$	$2_{xz}]$	
35	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{x}y}$	2_{xy}	4_z	$4_z^3]$	35	1	$\bar{1}2_{\bar{x}y}$						
36	1	2_x	2_y	$2_z+\bar{1}[2_{\bar{y}z}$	2_{yz}	4_x	$4_x^3]$	36	1	$\bar{1}2_{\bar{y}z}$						
45	1	2_x	2_y	2_z				45	1	$\bar{1}2_{xy}$						
46	1	2_x	2_y	2_z				46	1	$\bar{1}2_{yz}$						
56	1	2_x	2_y	2_z				56	1	$\bar{1}2_{xz}$						

is the point group of the bovine liver catalase molecules. While other choices of the rotation A could have been taken to define a test function $T(\mathbf{x},A)$, we have taken $A=\bar{4}_X$ since the peaks of $T(\mathbf{x},\bar{4}_X)$ are neither streaked nor smeared.

To calculate all peaks of the translation function $T(\mathbf{x},\bar{4}_X)$ one first determines the indices $jk,j'k'$ for which $\{A(jk,j'k')\}$ contains the rotation $\bar{4}_X$. The positions $\mathbf{x}$ of the peaks of $T(\mathbf{x},\bar{4}_X)$ are calculated from equations (9) and (10). The translation vectors can be written in terms of the molecular position $\mathbf{r}_1$ and the lattice parameters of the crystal. Therefore, the coordinates of the positions of the peaks can be calculated in terms of the unknown hexagonal coordinates (x_0,y_0,z_0) of the molecular position $\mathbf{r}_1$, and the parameters $c/3$ and $a/3$, where a and c are the lattice parameters of the hexagonal unit cell. That is, each of the three coordinates of a peak can be given by five numbers N_i, $i=1,2,\ldots,5$, and its numerical value by $x_0N_1+y_0N_2+z_0N_3+cN_4/3+aN_5/3$.

In Figs. 5 and 6, for $\mathbf{P}=222$ (D_2) and 4 (C_4), respectively, we have plotted the peaks of the translation function $T(\mathbf{x},\bar{4}_X)$ which lie on a subsection of the plane defined by the Z_H axis and the line $Y_H=2X_H$. That these peaks lie on this plane is not dependent on the numerical values of x_0, y_0, z_0, c and a. To represent the results of this calculation pictorally, *i.e.* to obtain numerical values of the positions of the peaks on this plane, we have used the values $x_0=110{\cdot}84$ Å, $y_0=24{\cdot}24$ Å, $z_0=11{\cdot}87$ Å (Barynin & Vainshtein, 1971) and $a=173{\cdot}3$ Å and $c=237{\cdot}4$ Å (Longley, 1967; Rossmann & Labaw, 1967; Vainshtein, Barynin, Gurskaya & Mikitin, 1967) to calculate the positions $\mathbf{x}$ of these peaks and the magnitude of $\mathbf{y}$ corresponding to each peak. We have plotted all positions $\mathbf{x}$ whose corresponding vector $\mathbf{y}$ is of magnitude of less than 200 Å, *i.e.* taking the radius of the volume U as 100 Å.

Comparing Figs. 5 and 6, one finds that all peaks of Fig. 6, where $\mathbf{P}=4$ (C_4) are contained in Fig. 5, where $\mathbf{P}=222$ (D_2). However, the translation function for $\mathbf{P}=222$ (D_2) contains many more peaks. Consequently, by calculating from experimental data the translation function $T(\mathbf{x},\bar{4}_X)$ for $\mathbf{x}$ lying on this special plane, one can determine which of the point groups, 222 (D_2) or 4 (C_4), is the point group of the bovine liver catalase molecules.

To determine the coordinates (x_0,y_0,z_0) of the molecular position $\mathbf{r}_1$, we first consider the case where $\mathbf{P}=222$ (D_2). One finds that all peaks, in Fig. 5, lie along seven lines parallel to the Z_H axis. We denote the intercepts of these lines with the X'_H axis, the coordinate axis perpendicular to Z_H lying in this plane, as $X'_H(i)$, $i=1,2,\ldots,7$, and list them in Table 5. One can distinguish these seven intercepts by noting that in general

$$X'_H(2)+X'_H(6)=X'_H(7)$$
$$X'_H(3)+X'_H(5)=X'_H(7)$$
$$X'_H(2)+X'_H(3)=X'_H(4)$$

and that the dominating peaks line on the lines which intersect the X'_H axis at $X'_H(2)$, $X'_H(4)$, and $X'_H(5)$. One can determine x_0 and y_0 from $X'_H(3)$ and $X'_H(6)$, since, see Table 5, $X'_H(3)=\sqrt{3}y_0$ and $X'_H(6)=\sqrt{3}x_0-\sqrt{3}a/3$. The component z_0 of $\mathbf{r}_1$ can be determined from the Z_H component of the dominating peak on the line

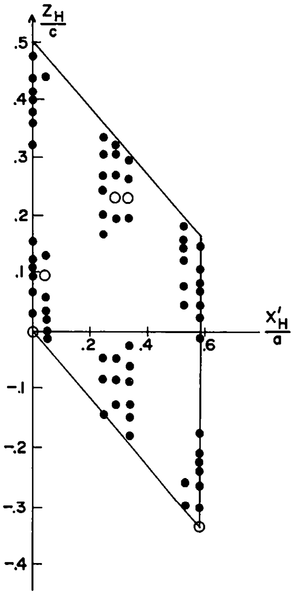

Fig. 5. Peaks of the translation function $T(\mathbf{x},4_X)$ lying on the $Z_HX'_H$ plane, where the X'_H axis is defined along the line $2X_H=Y_H$, for the model of trigonal crystalline bovine liver catalase where the point group of the molecules is 222 (D_2). Dominating peaks are denoted by open circles.

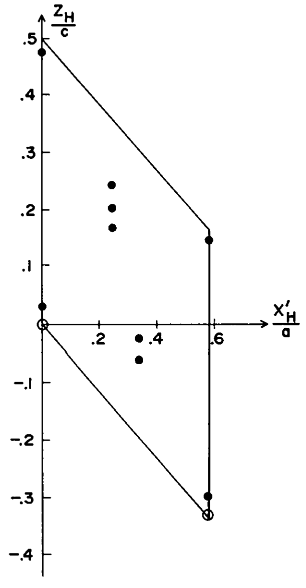

Fig. 6. Peaks of the translation function $T(\mathbf{x},\bar{4}_X)$ lying on the $Z_HX'_H$ plane for the model of trigonal crystalline bovine liver catalase where the point group of the molecules is 4 (C_4). Dominating peaks are denoted by open circles.

whose intercept is $X'_H(2)$, since the Z_H component of this peak is equal to $2z_0$. Knowing the components of $\mathbf{r}_1$, one determines the remaining molecular positions in the unit cell using equation (11).

Table 5. *The X'_H coordinate of the peaks of the translation function shown in Fig. 5, given by the expression $x_0N_1+y_0N_2+z_0N_3+cN_4/3+aN_5/3$, listed in terms of the values of the coefficients N_i, $i=1,2,\ldots,5$*

	X'_H				
	N_1	N_2	N_3	N_4	N_5
$X'_H(1)$	0	0	0	0	0
$X'_H(2)$	$-\sqrt{3}$	0	0	0	$2\sqrt{3}$
$X'_H(3)$	0	$\sqrt{3}$	0	0	0
$X'_H(4)$	$-\sqrt{3}$	$\sqrt{3}$	0	0	$2\sqrt{3}$
$X'_H(5)$	0	$-\sqrt{3}$	0	0	$\sqrt{3}$
$X'_H(6)$	$\sqrt{3}$	0	0	0	$-\sqrt{3}$
$X'_H(7)$	0	0	0	0	$\sqrt{3}$

In the case where $\mathbf{P}=4$ (C_4), one can determine from the peaks of the translation function shown in Fig. 6 only x_0 and y_0; $X'_H(3)=\sqrt{3}y_0$, and the Z_H component of the higher peak on the $X'_H(s)$ line is $-\sqrt{3}y_0/2+2z_0$. One cannot determine x_0 from the positions of the peaks in Fig. 6, since the numerical values of the positions of these peaks are independent of x_0.

To determine x_0, one could plot the translation function $T(\mathbf{x},\bar{4}_X)$ in the volume defined by $0<X_H/a\leq 1$, $0\leq Y_H/a\leq 1$, and $-0{\cdot}5\leq Z_H/a\leq 0{\cdot}5$. In Fig. 6 we show the positions of the strongest peaks, excluding those at $\mathbf{x}=\mathbf{t}$. These peaks lie in six planes perpendicular to the Z_H axis, and the intercepts of these planes with the Z_H axis, denoted by $Z_H(i)$, $i=1,2,\ldots,6$, are listed in Table 6. By determining, for example, $Z_H(1)$ one can determine x_0, since $Z_H(1)=-\sqrt{3}x_0/2+\sqrt{3}y_0/2-z_0-c/3+\frac{1}{2}(\sqrt{3}/2)a$, assuming that y_0 and z_0 have been previously determined from Fig. 7.

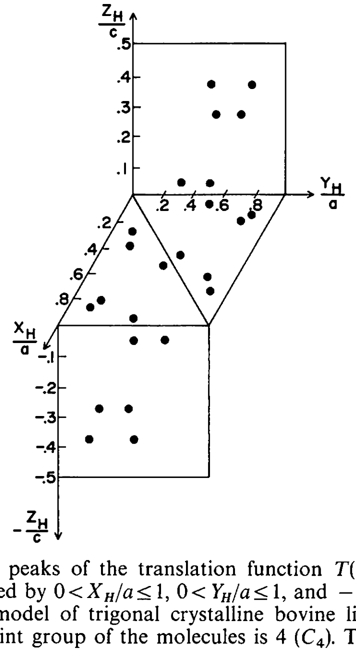

Fig. 7. Highest peaks of the translation function $T(\mathbf{x},\bar{4}_X)$ in the volume defined by $0<X_H/a\leq 1$, $0<Y_H/a\leq 1$, and $-0{\cdot}5\leq Z_H/c\leq 0{\cdot}5$, for the model of trigonal crystalline bovine liver catalase where the point group of the molecules is 4 (C_4). The Z_H components of peaks where $X_H>Y_H$ are negative, where $X_H<Y_H$, positive.

Table 6. *The Z_H coordinate of the peaks of the translation function shown in Fig. 7, given by the expression $x_0N_1+y_0N_2+z_0N_3+cN_4/3+aN_5/3$, listed in terms of the values of the coefficients N_i, $i=1,2,\ldots,5$*

In the right-hand column, the Z_H coordinate of $Z_H(i)$ is given in terms of the Z_H coordinate of $Z_H(1)$ and lattice parameter c of the hexagonal unit cell.

$Z_H(1)$	$-\sqrt{\frac{3}{2}}$	$\sqrt{\frac{3}{2}}$	-1	-1	$\frac{3}{2}\sqrt{\frac{3}{2}}$	
$Z_H(2)$	$\sqrt{\frac{3}{2}}$	$-\sqrt{\frac{3}{2}}$	1	-1	$-\frac{3}{2}\sqrt{\frac{3}{2}}$	$-Z_H(1)-\frac{2}{3}c$
$Z_H(3)$	$-\sqrt{\frac{3}{2}}$	$\sqrt{\frac{3}{2}}$	-1	0	$\frac{3}{2}\sqrt{\frac{3}{2}}$	$Z_H(1)+\frac{1}{3}c$
$Z_H(4)$	$\sqrt{\frac{3}{2}}$	$-\sqrt{\frac{3}{2}}$	1	0	$-\frac{3}{2}\sqrt{\frac{3}{2}}$	$-Z_H(1)-\frac{1}{3}c$
$Z_H(5)$	$-\sqrt{\frac{3}{2}}$	$\sqrt{\frac{3}{2}}$	-1	1	$\frac{3}{2}\sqrt{\frac{3}{2}}$	$Z_H(1)+\frac{2}{3}c$
$Z_H(6)$	$\sqrt{\frac{3}{2}}$	$-\sqrt{\frac{3}{2}}$	1	1	$-\frac{3}{2}\sqrt{\frac{3}{2}}$	$-Z_H(1)$

The author would like to thank Professor M. G. Rossmann for correspondence and conversations, and M. Kilian for assistance in computing Tables 1–4 of this paper.

This work was supported by a grant from the National Research Council of Canada.

APPENDIX I

In the case of a crystal consisting of identical molecules where the positions of the molecules in the unit cell constitute q sets of equivalent positions, the rotations which rotate a molecule into the orientation of another molecule are determined as follows (Litvin, 1975): Let $\mathbf{r}^\alpha_j=R^\alpha_j\mathbf{r}^\alpha_1+\boldsymbol{\tau}(R^\alpha_j)$ denote the position of the jth molecule in the αth set of equivalent positions, where $(R^\alpha_j|\boldsymbol{\tau}(R^\alpha_j))$ is an element of the space group of the crystal. Let $\mathbf{P}$ denote the point group of the molecule at $\mathbf{r}^1_1$, and for $\alpha=1,2,\ldots,q$, R^α a rotation which rotates the molecule at $\mathbf{r}^1_1$ into the orientation of the molecule at $\mathbf{r}^\alpha_1$. The set $\{R(\alpha j,\beta k)\}$ of rotations which rotate the molecule at $\mathbf{r}^\alpha_j+\mathbf{t}$ into the orientation of the molecule at $\mathbf{r}^\beta_k+\mathbf{t}'$ is given, in terms of $\mathbf{P}$, R^α, and R^α_j, by [compare with equation (7)]:

$$\{R(\alpha j,\beta k)\}=\{R^\beta_kR^\beta\mathbf{P}(R^\alpha_jR^\alpha)^{-1}\}.$$

Peaks of the translation function at $\mathbf{x}=(\mathbf{r}^\beta_k-\mathbf{r}^\alpha_j)+\mathbf{t}+\mathbf{y}$ where $\mathbf{y}-A\mathbf{y}=(\mathbf{r}^{\beta'}_{k'}-\mathbf{r}^{\alpha'}_{j'})-(\mathbf{r}^\beta_k-\mathbf{r}^\alpha_j)+\mathbf{t}'-\mathbf{t}$ [compare with equations (9) and (10) respectively] are associated with rotations contained in the set of rotations $\{A(\alpha j,\beta k;\alpha' j',\beta' k')\}$ given by [compare with equation (8)]:

$$\{A(\alpha j,\beta k;\alpha' j',\beta' k')\}=[\{R(\alpha j,\alpha' j')\}\cap\{R(\beta k,\beta' k')\}]$$
$$+\bar{1}[\{R(\alpha j,\beta' k')\}\cap\{R(\beta k,\alpha' j')\}].$$

APPENDIX II

The translation function $T(\mathbf{x},m)$, equation (2), was introduced by Rossmann *et al.* (1964). In that same paper, the general translation function $T(\mathbf{x},A)$, equation (3), was implicitly considered and rejected. We shall review here the derivative by Rossmann *et al.* in terms of the general theory of translation functions presented in this paper, and conclude that the erroneous rejection by these authors of the translation function $T(\mathbf{x},A)$, equation (3), was due to an error in mathematical logic.

In the terminology of this paper, Rossmann *et al.* (1964) restrict themselves to determining conditions on rotations A such that the translation function $T(\mathbf{x},A)$ has a peak at $\mathbf{x}=\mathbf{\Delta}_{jk}$. They consider only the array of cross-vectors $P_{jk0}(\mathbf{r})$ centred at $\mathbf{r}=\mathbf{\Delta}_{jk}$, and consequently were determining conditions that A is a rotation which leaves the array of cross-vectors $P_{jk0}(\mathbf{r})$ invariant. They derive the *sufficient* condition that if R is a rotation of 180° contained in $\{R(jk)\}$, then $A=\overline{R}\equiv m$. This sufficient condition follows directly from the general theory presented in this paper: $T(\mathbf{x},A)$ has a peak at $\mathbf{x}=\mathbf{\Delta}_{jk}$ if A is a rotation contained in $\{A(jk,jk)\}$, where from equation (8):

$$\{A(jk,jk)\}=[\{R(jj)\}\cap\{R(kk)\}] + \overline{1}[\{R(jk)\}\cap\{R(kj)\}].$$

If R is a proper rotation contained in $\{R(jk)\}$, R^{-1} is contained in $\{R(kj)\}$ (Litvin, 1975), and consequently if $R=R^{-1}$ (a rotation of 180° obviously satisfies this) then a rotation $A=\overline{R}$ is contained in $\{A(jk,jk)\}$.

Rossmann *et al.* (1964) then seem to interpret this sufficient condition as a *necessary* condition, conclude then that a rotation A not equal to m cannot leave the array of cross-vectors invariant, and subsequently reject the translation function $T(\mathbf{x},A)$, $A\neq m$, out of hand. Their erroneous interpretation of a sufficient condition as a necessary condition has led them to their erroneous conclusion.

References

Adams, M. J., Ford, G. C., Koekoek, R., Lentz, P. R. Jr, McPherson, A. Jr, Rossmann, M. G., Smiley, I. E., Shevitz, R. W. & Wonacott, A. J. (1970). *Nature, Lond.* **227**, 1098–1103.

Argos, A., Ford, G. C. & Rossmann, M. G. (1975). *Acta Cryst.* A**31**, 499–506.

Barynin, V. G. & Vainshtein, B. K. (1971). *Kristallografiya*, **16**, 751–763.

Blow, D. M., Rossmann, M. G. & Jeffery, B. A. (1964). *J. Mol. Biol.* **8**, 65–78.

Bricogne, G. (1974). *Acta Cryst.* A**30**, 395–405.

Bricogne, G. (1976). *Acta Cryst.* A**32**, 832–847.

Crowther, R. A. & Blow, D. M. (1967). *Acta Cryst.* **23**, 544–548.

Dobson, E., Harding, M. M., Hodgkin, D. C. & Rossmann, M. G. (1966). *J. Mol. Biol.* **16**, 227–241.

Eventoff, W. & Gurskaya, G. V. (1975). *J. Mol. Biol.* **93**, 55–62.

Fridborg, K., Hjerten, S., Höglund, S., Liljas, A., Lundberg, B. K. S., Oxelfelt, P., Philipson, L. & Strandberg, B. (1965). *Proc. Natl. Acad. Sci. US*, **54**, 513–521.

Glauser, S. & Rossmann, M. G. (1966). *Acta Cryst.* **21**, 175–176.

Gurskaya, G. V., Lobanova, G. M. & Vainshtein, B. K. (1971). *Kristallografiya*, **16**, 764–773.

Huber, R. (1969). *Crystallographic Computing*, edited by F. R. Ahmed, pp. 96–102. Copenhagen: Munksgaard.

Johnson, J. E., Argos, P., Rossmann, M. G. & Wagner, M. A. (1975). *Acta Cryst.* B**31**, 2577–2583.

Lattmann, E. E. & Love, W. E. (1970). *Acta Cryst.* B**26**, 1853–1857.

Lentz, P. J. & Strandberg, B. (1974). *Acta Cryst.* A**30**, 552–559.

Litvin, D. B. (1975). *Acta Cryst.* A**31**, 407–416.

Longley, W. (1967). *J. Mol. Biol.* **30**, 323–327.

Nordman, C. E. (1966). *Trans. Amer. Cryst. Assoc.* **2**, 29–38.

Rossmann, M. G. (1972). *The Molecular Replacement Method.* New York: Gordon and Breach.

Rossmann, M. G. (1973). *Trans. Amer. Cryst. Assoc.* **9**, 101–122.

Rossmann, M. G. & Blow, D. M. (1962). *Acta Cryst.* **15**, 24–31.

Rossmann, M. G., Blow, D. M., Harding, M. M. & Coller, E. (1964). *Acta Cryst.* **17**, 338–342.

Rossmann, M. G. & Labaw, L. W. (1967). *J. Mol. Biol.* **29**, 315–316.

Tollin, P. (1966). *Acta Cryst.* **21**, 613–614.

Tollin, P. (1969). *J. Mol. Biol.* **45**, 481–490.

Tollin, P. & Cochran, W. (1964). *Acta Cryst.* **17**, 1322–1324.

Vainshtein, B. K., Barynin, V. V., Gurskaya, G. V. & Mikitin, B. La. (1967). *Kristallografiya*, **12**, 860–867.