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Remarks on the Delaunay Reduction

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Delaunay's reduction of a primitive cell to a standard form is summarized with emphasis on important points which have been omitted in the current accounts of his work. A new reduction is introduced which has the same object as that of Delaunay but which is more rapidly convergent though less general. The counterpart of the Delaunay reduction in reciprocal space is also investigated and comment is made on the relation of the Delaunay standard form to others which have been suggested.

Introduction

In a very important paper in the field of lattice geometry, Delaunay (1933, referred to as Delaunay) set up a method for the reduction of the most general primitive cell of any lattice to a standard form involving four vectors which make obtuse angles with one another. Any three of these four vectors form a primitive triplet of the lattice if the original cell is primitive. Delaunay also presented tables which permit the recognition of the symmetry properties of the lattice in the reduced set. The power of Delaunay's reduction and the degree of uniqueness which can be achieved with its aid make it an ideal basis for the establishment of a cataloguing system for crystal lattice cell dimensions.

The reduction method has been described and used by Donnay (in Donnay & Nowacki, 1954, referred to as Donnay) as a basis for a table of triclinic cell dimensions. Accounts of the method have also been given by Ito (1950, referred to as Ito) and in the *International Tables for X-ray Crystallography* (1952, referred to as *ITXC*). It is unfortunate, however, that no one of these descriptions of the method is sufficient to permit the completion of the Delaunay reduction.

In the following section the main points of Delaunay's paper are summarized. Special emphasis is laid on the ambiguities of the reduction, well recognized by Delaunay but omitted from the discussions of the later writers. In later sections, a new reduction is introduced which is of less general applicability than that of Delaunay but which increases the rate of convergence to the same final result. Comment is also made on the counterpart of the Delaunay reduction in reciprocal space and on the relationship of the Delaunay reduced cell to that having the shortest three non-coplanar translations.

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Description of the Delaunay reduction

The reduction starts with any primitive triple $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ and adds to it a fourth vector $\mathbf{b}_4 = -\mathbf{b}_1-\mathbf{b}_2-\mathbf{b}_3$. It then proceeds, by a series of steps, to transform these four vectors to a set $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4$ for which the six scalar products $g_{ij} = (\mathbf{a}_i\mathbf{a}_j)$, $i \neq j$, are all negative or zero. A single step of the reduction is indicated in Fig. 1(*a*, *b*), where the scalar products of the set $\mathbf{b}_i$ are indicated by $h_{ij} = (\mathbf{b}_i\mathbf{b}_j)$, and are written sche-

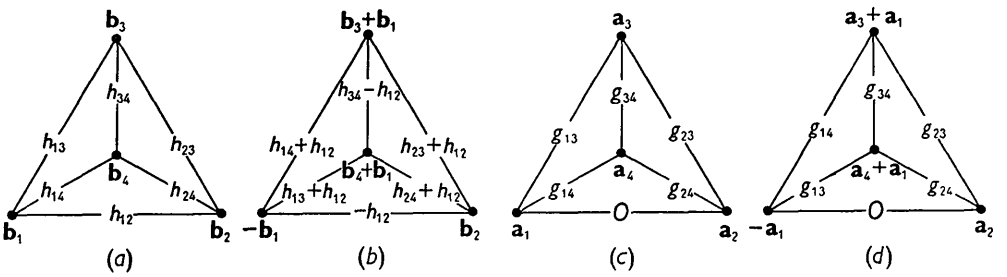

Fig. 1. (*a*, *b*) A single step in the Delaunay reduction. Notation: $h_{ij} = (\mathbf{b}_i\mathbf{b}_j)$. The scalar product $h_{12} = (\mathbf{b}_1\mathbf{b}_2)$ is assumed to be positive in (*a*). It is made negative in (*b*) by changing the sign of $\mathbf{b}_1$, leaving $\mathbf{b}_2$ unchanged, and adding $\mathbf{b}_1$ to $\mathbf{b}_3$ and $\mathbf{b}_4$. The scalar products for the new set are as indicated in (*b*): i.e. h_{12} is subtracted from h_{34} and added to h_{23} and h_{24} and to the interchanged pair h_{14} and h_{13}. (*c*, *d*) Two ambiguous cases for $g_{12} = 0$ in the triclinic system obtained by 'changing the sign' of the zero product.

matically on the edges of a tetrahedral symbol. Note that

$$h_{ii} = -(h_{ij}+h_{ik}+h_{il}), \quad i,j,k,l = 1,2,3,4\,. \quad (1)$$

An important check is provided by Delaunay's remark that the negative sum of the scalar products decreases at each step by the magnitude of that product whose sign is changed. Thus in Fig. 1(*a*), the negative sum of the scalar products is the positive number

$$\Sigma_1 = \tfrac{1}{2}(h_{11}+h_{22}+h_{33}+h_{44}) = -(h_{12}+h_{23}+h_{31}+h_{14}+h_{24}+h_{34})\,, \quad (2)$$

while in Fig. 1(*b*) this sum has decreased to

$$\Sigma_2 = -(2h_{12}+h_{23}+h_{31}+h_{14}+h_{24}+h_{34})\,. \quad (3)$$

Thus the decrease in Σ is

$$\Sigma_1-\Sigma_2 = h_{12}\,. \quad (4)$$

The reduction is repeated until all scalar products are either negative or zero. Delaunay shows that there are twenty-four basic forms which the reduced set may take and exhibits a table of these forms indicating their relationship to the fourteen Bravais lattices. Modified and amplified forms of this table have been presented by Ito and *ITXC**.

Delaunay presents an argument by exhaustion to show that, in the case in which all scalar products are non-zero, the reduced form is unique. He also points out that in the cases in which zero values occur the reduction is ambiguous, since one can then alter the arrangement of the products in the tetrahedron, and hence the vectors in the reduced set, without changing the quantity (2). This operation is of course carried out by 'changing the sign' of the zero terms.

There are two ways in which the presence of a zero may be important in the final reduction: (i) It may lead to an ambiguity in the choice of cell. (ii) It may lead to a symmetry pattern which is not recognized as one of the twenty-four tabulated by Delaunay, Ito, and *ITXC*.

The first difficulty is most important in the triclinic system and is illustrated in Fig. 1(*c*, *d*). If we assume that Fig. 1(*c*) (or one of its permutations under the symmetry of the reduction) is the first reduced configuration, then by changing the sign of the zero product we obtain the configuration of Fig. 1(*d*). In the first case, the possible base vectors have magnitudes that are the square-roots of the quantities:

$$g_{11} = -(g_{13}+g_{14});\quad g_{22} = -(g_{23}+g_{24});$$
$$g_{33} = -(g_{13}+g_{23}+g_{34});\quad g_{44} = -(g_{14}+g_{24}+g_{34}).$$

In the second case, the corresponding values are:

$$h_{11} = g_{11};\quad h_{22} = g_{22};\quad h_{33} = -(g_{14}+g_{23}+g_{34});$$
$$h_{44} = -(g_{13}+g_{34}+g_{24})$$

and we note that:

$$h_{33} = g_{33}+g_{11}+2g_{13};\quad \text{and}\quad h_{44} = g_{44}+g_{11}+2g_{14}\,.$$

It is thus possible that the shortest three non-coplanar translations with a tri-obtuse cell may not occur in the first reduced quadruple which is obtained after a Delaunay reduction, but may occur only after one or more changes of the sign of zero. Practical examples of this situation are readily obtained from the Donnay tables. The two entries for wollastonite (T:0·773 and T:0·923) are related by the transformation which we have just described. Clearly the second of these has the smaller primitive translations. There is an alternative cell for pectolite (T:0·757) which has a shorter b translation than that of the setting given by Donnay. There are alternative settings for cyclohexane nitrosite (T:0·705), kaolinite (T:0·825), and aramayoite (T:0·949), but in each case the cell presented in the tables is that with the shorter translations.

In those cases in which two scalar products are zero, there are three alternative quadruples which can easily be found by the reader. We have found a case of this type in Donnay's tabulation: i.e. parahilgardite (T:0·504). There are clearly other entries in the table which are subject to the same general type of ambiguity, but we have not attempted a complete discussion of them.

In the monoclinic primitive cases there are two zeros on adjacent edges of the tetrahedron and no equalities among the remaining products. There are then three reduced cases and only in one of these will the least two translations in the **ac** net be exhibited. No attempt has been made to search for such cases in the Donnay tabulation and none is expected because a special reduction for the monoclinic system was used.

In the monoclinic centered lattices caution must be exercised in using Table 5·1·1 of *ITXC* in the choice of cell translations since in addition to the ambiguities now under discussion there are also possible ambiguities in allotting the symbols in the formulae and diagrams of the table to a given numerical example. In these cases and in the primitive and centered lattices of symmetry higher than monoclinic (where the choice of cell translations should offer no problem) difficulty may arise for the second reason cited above, i.e. that one or more changes of sign of zero may be necessary before the symmetry pattern is exhibited in the form in which Delaunay tabulated it. This, of course, was recognized by Delaunay but was not discussed by Ito and *ITXC*. The ambiguous cases are exhibited in Fig. 2(*a*), which is essentially an amplification of the two text figures at the top of p. 136 of Delaunay's paper.

A practical example of the situation envisaged in the present discussion is presented by the lattice worked out by Ito. He obtains a presentation of the lattice *Cmmm* in one of its forms. The other configuration exhibited in Fig. 2(*a*) could equally well have been obtained by a different manipulation of the

* Note that in *ITXC*, Table 5·1·1 (pp. 534–5), the figures for the second and sixth monoclinic cases should be interchanged. The limiting ranges for several of the cases are incorrectly stated, but this does not affect the use of the table.

original data, and a difficulty would then have been encountered in its interpretation.

In all lattices, other than those referred to above, the alternative settings produced by change of sign of zero will correspond merely to a change among the equivalent primitive cells to which the lattice may be referred. The example discussed in *ITXC* is of this type.

Another point made by Delaunay which has not been emphasized by the later writers is that the symmetry of the twenty-four standard forms is minimal. Extra equalities between products may occur without changing the standard form provided that the added symmetry is not that required by another standard form. This situation is illustrated by Fig. 2(*b*) in which all the possible equalities for two adjacent zero products are exhibited.

We have investigated all possibilities and have found that there are 72 cases which exhibit zeros and equalities in arrangements which are different under the tetrahedral group. All of them can be shown to be specializations of the 24 cases of Delaunay. These need not be presented in detail here since they can be easily derived and are of little importance provided that the point mentioned in the first two sentences of the preceding paragraph is kept in mind.

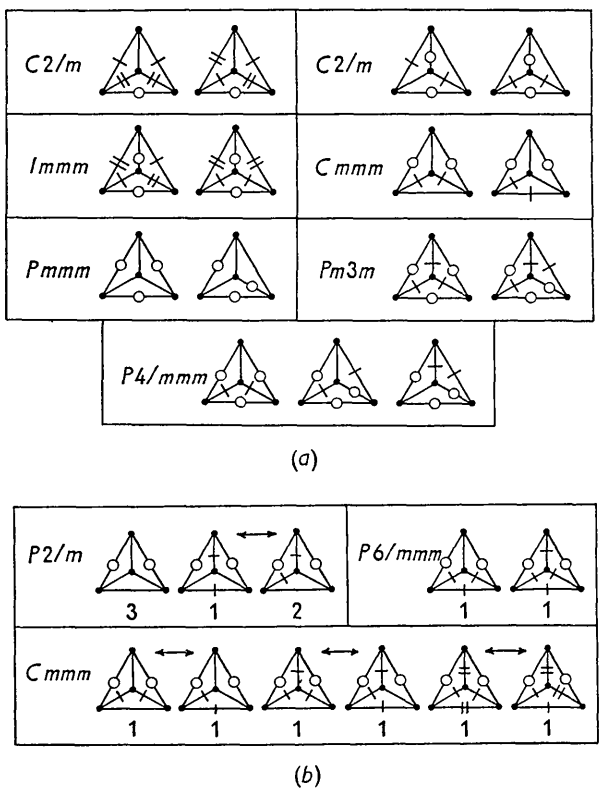

Fig. 2. (*a*) Alternative presentations of the symmetrical cases which may appear as a result of a Delaunay reduction. These alternatives transform into one another by changes of sign of zero. The space-group symbols correspond to the Laue groups of the lattices in question. (*b*) Examples (for the cases with two adjacent zeros) of added symmetry which does not change the standard form. In each box the tabulated standard form is given on the left. Forms which are related by a zero transformation are connected by double arrows. The number beneath each symbol indicates the number of non-equivalent cells of the same symmetry which may be obtained from it by a zero transformation.

It is worthwhile mentioning that when the initial cell is badly misset the Delaunay reduction may take many steps. It is therefore important to choose a reasonable cell in preparing the original data, and teachers of crystallography should exercise caution in devising examples for reduction by their students. It is difficult to formulate rules for the best procedure in the reduction. The form of the expression (2) would suggest that it is always best to work with the largest term and this is undoubtedly correct in the earlier stages of the reduction. In the later stages, it is perhaps better to choose a move which does not unduly increase the magnitude of the terms which are already negative.

Since the order in which steps are taken in the reduction will not affect the end result, except as to setting, and will merely concern the rate of convergence, the routine seems ideally adapted for machine computation.

An alternative reduction

The approach to the end point of a Delaunay reduction may often be accelerated by using the alternative reduction shown in Fig. 3. In this reduction two

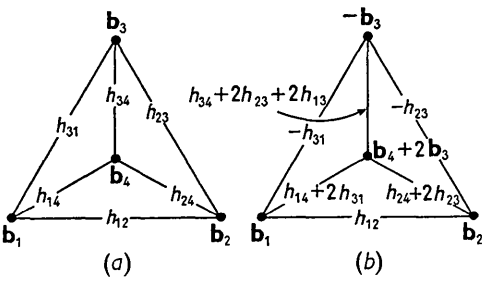

Fig. 3. An alternative reduction (the notation is that of Fig. 1(*a*, *b*)). The sum $h_{23}+h_{31}$ is assumed to be positive in (*a*). The signs of these two terms are changed in (*b*) by changing the sign of $\mathbf{b}_3$ and adding twice $\mathbf{b}_3$ to $\mathbf{b}_4$, $\mathbf{b}_1$ and $\mathbf{b}_2$ being unchanged. The scalar products for the new set are as indicated in (*b*): i.e. h_{31} and h_{23} are changed in sign, while h_{12} is unchanged. The three changed products are $h_{14}+2h_{31}$, $h_{24}+2h_{23}$, $h_{34}+2h_{23}+2h_{13}$.

vectors are kept constant and the sign of a third is changed, with the addition of twice the changed vector to the fourth. The changes in the scalar products are given in the figure. With this reduction, the change in Σ (cf. equation (4)) is

$$\Sigma_1-\Sigma_2 = 2(h_{23}+h_{31}) . \qquad (5)$$

Thus this transformation is very much more effective than that of Fig. 1(*a*, *b*). It should always be used when two adjacent products are both positive. It can

Table 1. *Tri-acute cell with shortest three non-coplanar translations*

Case	Vectors	Condition	Transformation
1	$\mathbf{a}_1+\mathbf{a}_2$ replaces $\mathbf{a}_2$	$-g_{12} < -(g_{13}+g_{14})$	$\mathbf{A}_1 = -\mathbf{a}_1;\ \mathbf{A}_2 = -\mathbf{a}_1-\mathbf{a}_2;\ \mathbf{A}_3 = \mathbf{a}_3$
2	$\mathbf{a}_2+\mathbf{a}_3$ replaces $\mathbf{a}_3$	$-g_{23} < -(g_{21}+g_{24})$	$\mathbf{A}_1 = \mathbf{a}_1;\ \mathbf{A}_2 = -\mathbf{a}_2;\ \mathbf{A}_3 = -\mathbf{a}_2-\mathbf{a}_3$
3	$\mathbf{a}_3+\mathbf{a}_1$ replaces $\mathbf{a}_3$	$-g_{13} < -(g_{12}+g_{14})$	$\mathbf{A}_1 = -\mathbf{a}_1;\ \mathbf{A}_2 = \mathbf{a}_2;\ \mathbf{A}_3 = -\mathbf{a}_1-\mathbf{a}_3$

be used with profit when only one (say h_{23}) is positive provided that the sum $h_{23}+h_{31}$ is greater than one-half of h_{23}. We have called the reduction of Fig. 3 a 'double reduction'.

The cell with the shortest three non-coplanar translations

As Delaunay pointed out, the reduced cell is not necessarily the cell with the shortest three non-coplanar translations. If the cell with the shortest three translations is tri-obtuse (cf. Donnay, 1943), it will be given directly by the Delaunay reduction. If that cell is tri-acute, at least two of the shortest three translations will appear in the reduced quadruple and the third will be one of the diagonals $\mathbf{a}_1+\mathbf{a}_2$, $\mathbf{a}_2+\mathbf{a}_3$, $\mathbf{a}_3+\mathbf{a}_1$ in the ordered quadruple $(a_1 \leq a_2 \leq a_3 \leq a_4)$. The three cases which can arise are indicated in Table 1, which includes the conditions under which the diagonal vectors replace vectors of the original quadruple in forming the tri-acute cell. It may interest the reader to convince himself that the transformations of Column 4 of the table may be obtained on the Delaunay tetrahedral diagram by first changing the sign of $\mathbf{a}_1$ in such a manner as to retain $\mathbf{a}_2$ or $\mathbf{a}_3$ as required and at the same time to exhibit the required diagonal. The second step then consists of a double reduction to make the three scalar products positive, and possibly an inversion if it is necessary to correct the hand of the axial system.

It is obvious that if there are zero scalar products in the reduced set, the cell with the shortest three translations can be presented as either non-acute or non-obtuse. Another more serious ambiguity arises when all scalar products are non-zero, and equalities appear in the Column 3 of the table. In such cases, there will be a tri-acute *and* a tri-obtuse cell with the shortest three translations.

The counterpart of the Delaunay reduction in reciprocal space

If we form the triple reciprocal to any three of the four vectors of a Delaunay reduced set, then this triple will be non-obtuse since we know that the angles in the reciprocal lattice for a non-acute cell in crystal space cannot be obtuse (cf. Buerger, 1942). The tetrahedron defined by these three reciprocal vectors then has the property that every one of its vertices projects orthogonally within or on the boundary of its opposite face, and the same tetrahedron or its inverse is obtained when any three of the four Delaunay reduced vectors are chosen. We have called such a tetrahedron 'compact'. It is clear that there is a one-to-one correspondence between the Delaunay reduced vectors in crystal-lattice space and the faces of the compact tetrahedron in reciprocal space. If the Delaunay reduction is unique, as it is when there are no right angles between the reduced vectors, the compact tetrahedron in reciprocal space will also be unique. If there are several Delaunay reduced sets in the crystal lattice corresponding to zero values of scalar products there will be corresponding compact tetrahedra in the reciprocal lattice. The compact tetrahedron is the Voronoi tetrahedron L_1 referred to by Delaunay (p. 146). It may be, but it is not necessarily, the principal tetrahedron as defined by Bravais (1850, pp. 54–7).

The importance of the idea of the compact tetrahedron lies in the fact that the latter can often be recognized directly in a stack of layers obtained from a series of reciprocal-lattice photographs made on the de Jong–Bouman (1938) retigraph or the Buerger (1942, 1944) precession camera; or in a set of sketches of reciprocal-lattice nets made from data obtained by other methods.

In a stack of photographs of the layers of a prominent zone, one tetrahedron will be apparent, as for example the tetrahedron *ABCD* of Fig. 4, in which

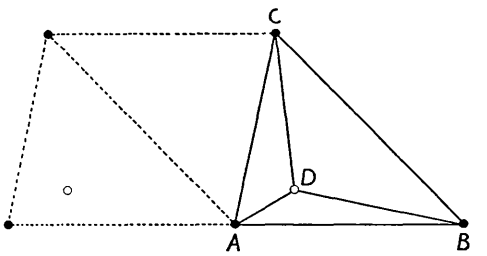

Fig. 4. Discussion of compact tetrahedron in reciprocal space.

the base *ABC* is one of the two congruent principal triangles of the net on which the stack is based and the vertex *D* projects inside or on the edge of the base and is a lattice point of the net next above that containing the base*. This tetrahedron will be a compact tetrahedron if the dihedral angles *DA*, *DB*, *DC* are all non-obtuse. This fact can be verified by calculation, but if, as is usual, a second stack based, say, on the *DAB* net is taken and the vertex *C* falls within the base, it only remains possible that the *CD* edge could be obtuse. If *C* does not fall within *DAB* in the new stack, obviously a new choice *C'* which does will give

* Note that the present discussion refers only to a general region of the reciprocal lattice in which no systematic absences due to glide planes or screw axes occur.

a tetrahedron which is more nearly compact than the one first chosen. It is easy to see that this process of 'rolling' a tetrahedron in reciprocal space is equivalent to one or more Delaunay reductions in crystal space.

We do not advocate the use of this process as a replacement of the Delaunay reduction but merely suggest that even a partial use of the concept of the compact tetrahedron in the choice of suitable reciprocal vectors will lead to a set of lattice vectors which are either Delaunay reduced or only a few steps removed from a Delaunay reduced set.

The two-dimensional analogue of the Delaunay reduction

The reduction of a two dimensional net to the obtuse-angled cell having the shortest two translations is simple enough when a scale drawing is made, but from numerical data the reduction may be cumbersome. Donnay has provided a nomogram for this reduction. There is, however, a numerical method for the reduction for the two-dimensional net which is strictly analogous to the Delaunay reduction for three-dimensional lattices. The scheme for this reduction is given in the caption of Fig. 5. and need not be repeated in

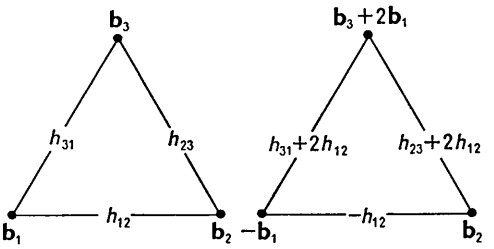

Fig. 5. Two-dimensional analogue of the Delaunay reduction. The sign of h_{12} is reversed by changing the sign of the vector $\mathbf{b}_1$, keeping $\mathbf{b}_2$, and adding $2\mathbf{b}_1$ to $\mathbf{b}_3$. The new products are obtained by adding twice the product which is reversed to the other two.

the text. The squared magnitude of any Delaunay vector is again given by the negative sum of the products which meet at a corner of the triangle. Note also that the quantity

$$\sigma = \tfrac{1}{2}(a_1^2+a_2^2+a_3^2) = -(g_{12}+g_{23}+g_{31})$$

is minimized by this reduction. Since only one of the three quantities g_{ij} can be negative, there is no choice to be made except for the two equivalent possibilities of choosing either of the two vectors entering into a product for reversal.

Discussion

There are two possible purposes to be served by a conventional 'setting' for crystal cell dimensions. The first is to provide a basis for a catalogue of crystal data. The second is to provide a standard framework for the presentation of the results of crystallographic investigations. When the only possible result of a crystal study was a description and a sketch of its external forms a standard presentation seemed possible. We now know that to present the results of a structure study we need various sections and projections, and that the choice of these sections and projections must be dictated by the actual structure rather than by convention. Granted, therefore, that no one standard setting will be adequate for the presentation of structural data, the question of the choice of a set of criteria for catalogue purposes should not be biased by pictorial considerations.

For catalogue purposes alone a set of rules is required which will identify a unique entry for a crystal cell. This entry may be accompanied by a small number of cross-references to take care of differences in the accuracy of the data possessed by the user and the compiler of the tables, and to take care of the fact that a crystal of low symmetry may have the lattice dimensions of one of a higher symmetry.

Two proposals of criteria for a conventional cell have received the most discussion: (*a*) the cell with the shortest three non-coplanar translations; (*b*) the cell which has as its translations the shortest three translations of the Delaunay reduced quadruple*. Clearly either of these criteria as stated will lead to ambiguous cases, but under either criterion an investigation of all possible ambiguities can be made to lead to a set of rules for their resolution. Delaunay has provided a simple algorithm for reaching his reduced quadruple and has given a complete account of the ambiguities involved in this procedure. The only other ambiguity which can arise in applying the second criterion appears when two or more of the translations of the reduced quadruple are equal in length, and this ambiguity can readily be removed by appropriate rules†. No complete investigation of the ambiguities for the first criterion has as yet been made, and no algorithm has been presented for the reduction of data. We have made a partial study of this problem and have shown how the cells appropriate to the first classification can be obtained from the Delaunay quadruple. We have also considered some of the ambiguities which arise, but our investigation is far from complete. Until such a study is completed the first criterion cannot be seriously supported as a basis for the classification of crystal data.

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* The recent proposal of Balashov (1956) is a mixture of the two. He suggests the use of the tri-obtuse cell with the shortest three non-coplanar translations, but his criteria for the tri-acute cases do not always lead to the tri-acute cell with the shortest three translations.

† We are indebted to Prof. Jürg Waser for pointing out to us the necessity for this remark.

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An Efficient Process for Solving Crystal Structures by Sign Relationships

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It is shown that, by expressing sign relationships in a suitable tabular form, it is possible to deduce signs for other structure factors if the signs are known for the structure invariants (the structure factors of even indices whose signs do not vary with the choice of origin of the unit cell). The economy introduced by considering only the structure invariants as unknowns, and not all the structure factors, makes possible the determination of reasonably complex structures by hand calculation. The application of the method to the structure of azo-benzene 2-sulphenyl chloride is described.

1. Introduction

The role of direct methods, which make use of sign relationships for solving crystal structures, is becoming progressively more important in crystallography but it would be fair to say that, at the present time, they do not seriously challenge older methods in achievement. Almost all the structures which have been solved by direct methods would have yielded to some other method, but the converse is certainly not true. However, direct methods do have the important virtue that they may often be tried fairly quickly, and failure is not too costly in time.

The present paper describes an efficient, systematic process by which sign relationships may be applied to the solution of crystal structures. With the aid of electronic computers the process should be capable of application to structures outside the scope of other direct methods hitherto reported.

2. The basis of the method

The discussion of this section will, for simplicity, be restricted to two dimensions, although the method can be applied in three dimensions. The $hk0$ projection of salicylic acid (two-dimensional space group *pgg*) will be used as an example of the application of the method. The reflexions considered are those of large unitary structure factor which were used by Cochran & Douglas (1954).

The reflexions are divided into the following four groups:

(*a*) h even, k even;
(*b*) h odd, k odd;
(*c*) h odd, k even;
(*d*) h even, k odd .

The signs of the reflexions of group (*a*) are indicated by the symbols a_1, a_2, etc., those of group (*b*) by b_1, b_2, etc., and so on. For salicylic acid we shall first consider only groups (*a*) and (*c*), for which the symbols and their significance are listed below.

$a_1 = s(10, 4)$	$c_1 = s(3, 12)$
$a_2 = s\ (4, 6)$	$c_2 = s(3, 2)$
$a_3 = s\ (2, 12)$	$c_3 = s(1, 6)$
$a_4 = s\ (2, 10)$	$c_4 = s(7, 2)$
$a_5 = s\ (6, 2)$	$c_5 = s(3, 6)$
$a_6 = s\ (2, 4)$	$c_6 = s(5, 4)$
$a_7 = s\ (2, 6)$	$c_7 = s(9, 4)$
$a_8 = s\ (4, 0)$	
$a_9 = s\ (6, 0)$	

where $s(h, k)$ denotes the sign of the reflexion $hk0$. The signs of a_8 and a_9 are found from inequalities to be + and − respectively.

All the sign relationships are now sought which relate one member of group (*a*) with two of group (*c*) and it is found that the following products are probably positive:

$-a_1c_4c_5$	$-a_7c_4c_7$	$-a_5c_3c_6$
$a_1c_2c_4$	$a_7c_1c_3$	$-a_7c_4c_6$
$-a_2c_1c_3$	$a_8c_2c_4$	$-a_4c_5c_6$
$-a_3c_3c_5$	$a_6c_2c_3$	$a_5c_5c_7$
$a_5c_2c_7$	$-a_7c_2c_6$	$a_8c_6c_7$