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The Choice of the Standard Unit Cell in a Triclinic Lattice

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An algorism for the reduction of the experimental data directly to the three shortest non-coplanar translations (Dirichlet triplet) is given. A method is also given for deriving the Dirichlet triplet from the Delaunay reduced cell, and analysis of the latter concept shows that the Delaunay cell can have interaxial angles arbitrarily near to 180°. For the Dirichlet triplet, in contrast, the interaxial angles can never deviate by more than 30° from right angles.

1. Introduction

In crystallography the choice of a unit cell in a lattice is, by convention, governed by the properties of symmetry. This applies to all crystallographic systems except the triclinic, where symmetry gives us no guidance.

Delaunay (1933) has given a profound and illuminating discussion of the geometry of crystal lattices, basing his work on the work of Selling (1874) and Voronoi (1908) on the reduction of positive definite quadratic forms. Delaunay makes great use of the 'Voronoi domains' (for definition see below, following equation (1·6)).

The lack of uniformity in the presentation of the lattice parameters of triclinic substances was realised long ago, and a number of suggestions were brought forward for a unique choice of the unit cell (Balashov, 1956; Barth & Tunell, 1933; Buerger, 1937, 1942, chap. 19, 1956, pp. 107–8); Crowfoot, 1935; Donnay & Melon, 1933; Donnay, Tunell & Barth, 1934; Donnay, 1943*a*, *b*, 1952; Peacock, 1937; Tunell, 1933). A particular cell, called the 'Delaunay reduced cell', brought to the attention of crystallographers by Ito (1950, p. 189), was later described in *International Tables* (1952, p. 530) and used by Donnay & Nowacki (1954) as a standard reference cell.

This cell is obtained from an arbitrary primitive cell by a simple and elegant algorism given by Delaunay (1933) and applied to the parameters of Selling. These refer to a quartet

$$\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d} \tag{1·1}$$

of lattice translations, satisfying

$$\mathbf{a}+\mathbf{b}+\mathbf{c}+\mathbf{d} = \mathbf{0}\,, \tag{1·2}$$

and such that any three of them form a primitive triplet. The Selling parameters are the six scalar products

$$\mathbf{a}.\mathbf{b}, \mathbf{a}.\mathbf{c}, \mathbf{a}.\mathbf{d}, \mathbf{b}.\mathbf{c}, \mathbf{b}.\mathbf{d}, \mathbf{c}.\mathbf{d}\,, \tag{1·3}$$

which are sufficient to determine the lengths of $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ and the angles between them: for

$$a^2 = \mathbf{a}.\mathbf{a} = -\mathbf{a}.\mathbf{b}-\mathbf{a}.\mathbf{c}-\mathbf{a}.\mathbf{d}\,, \tag{1·4}$$

$$ab\cos\gamma = \mathbf{a}.\mathbf{b}\,. \tag{1·5}$$

Selling's reduction theory shows that there is a particular quartet (1·1) of lattice vectors satisfying (1·2) and such that all the numbers (1·3) are negative or zero. In general the reduced quartet is unique (save for a possible *simultaneous* change of sign of all four) and gives Selling parameters all negative.

The so-called Delaunay reduced cell is formed from the reduced quartet ($\mathbf{a}_r, \mathbf{b}_r, \mathbf{c}_r, \mathbf{d}_r$) by discarding one of them, say $\mathbf{d}_r$, and taking the other three as concurrent edges of a parallelepiped. Whichever one of the quartet is discarded, this gives an 'obtuse parallelepiped', i.e. one having the three face-angles at one corner all obtuse. It appears to be usual to discard the *longest* vector of the reduced quartet.

From the definition it follows that the 'Delaunay' cell may reject a shorter lattice translation in favour of one much longer and there are cases in which even the shortest edge of the Delaunay cell is more than twice as long as a discarded translation, e.g. methylene blue iodide trihydrate. The data for this and some other substances are given as illustrations in Table 2 below.

At the same time, the obtuse angles of the 'Delaunay' cell may be very obtuse indeed, reaching 155° in the case quoted.

There is no theoretical limit to these effects. Space lattices exist (mathematically) for which the ratio of the shortest edge of the Delaunay cell to the shortest translation in the lattice is as large as we please, and for which one of the face angles of the Delaunay cell is as near to 180° as we please*. One may predict with confidence that crystalline substances will be encountered in nature which give Delaunay cells even more obtuse than our illustrations.

It therefore seems to us reasonable to draw attention to the more compact reduced cell of Dirichlet (1850); see also Niggli (1928, p. 111). This cell has three shortest translations for its edges and its axial angles cannot deviate by more than 30° from right angles.

The figures at the end of Table 2 show that the Dirichlet cell is obtained more easily than the Delaunay cell from the data published.

There is another argument in favour of the Dirichlet cell rather than the Delaunay one as a standard reference cell. With the Delaunay cell as standard, a cell with angles (say) 100°, 110°, 90°3′ is to be accepted, but one with angles 100°, 110°, 89° 57′ is to be rejected. We believe that the number of doubtful cases, and of cases in which thermal changes tilt the balance, is going to be greater if the Delaunay cell is used as standard than if the Dirichlet cell is adopted: certainly *Crystal Data* (Donnay & Nowacki, 1954) shows quite a significant number of triclinic substances with angles which have not been distinguished from 90°.

For this reason we shall give in § 3 an alternative algorism leading directly to the Dirichlet cell, and in § 4 rules for obtaining the Dirichlet cell from the Delaunay one, where these are distinct.

The relation between these two cells may also be expressed in terms of the Voronoi domains of the lattice. Given a lattice of points

* Starting with three mutually perpendicular vectors **a**, **b**, **c**, we can by slightly tilting them ensure that the Selling reduced quartet is

$$\mathbf{c}-\mathbf{a},\ \mathbf{a}-\mathbf{b},\ \mathbf{b},\ -\mathbf{c}\,.$$

If now **a** is very short compared with **b** and **c**, the Delaunay cell will have a face angle nearly 180°.

$$\mathbf{r} = \mathbf{r}_{uvw} = u\mathbf{a}+v\mathbf{b}+w\mathbf{c}\,, \tag{1·6}$$

where u, v, w run through all integer values, one attaches to each lattice point $\mathbf{r}_{uvw}$ the domain V_{uvw} of points which are nearer to $\mathbf{r}_{uvw}$ than any other lattice point. It is clear that the domains V_{uvw} do not overlap, fill space, are mutually congruent, and all have the same orientation. Quite apart from reasons of pure mathematics, there are physical reasons for treating V_{uvw}: for example, in many pure metals V_{uvw} is evidently the region of space in which the influence of the atom at $\mathbf{r}_{uvw}$ predominates (cf. Motsok (1929) on the relation between the lattice, the corresponding space-filling polyhedra, and the approximate 'shape' of the atom).

In general, a Voronoi domain is bounded by seven pairs of parallel planes: these are normal to the seven vectors

$$\mathbf{a}_r,\ \mathbf{b}_r,\ \mathbf{c}_r,\ \mathbf{d}_r\,, \tag{1·7}$$

$$\left.\begin{aligned} \mathbf{b}_r+\mathbf{c}_r &= -\mathbf{a}_r-\mathbf{d}_r\,,\\ \mathbf{c}_r+\mathbf{a}_r &= -\mathbf{b}_r-\mathbf{d}_r\,,\\ \mathbf{a}_r+\mathbf{b}_r &= -\mathbf{c}_r-\mathbf{d}_r\,. \end{aligned}\right\} \tag{1·8}$$

The edges of the Dirichlet cell are in fact the three shortest non-coplanar of these seven vectors and at most one of the three comes from (1·8). The edges of the Delaunay cell are the three shortest of the four vectors from (1·7), and in terms of them the various faces, etc., of the Voronoi domains may be expressed *algebraically* without having recourse to different algebraic forms in different cases. Thus (being necessarily centrosymmetrical) the faces of a Voronoi domain normal to the vectors (1·7) are hexagons and those normal to the vectors (1·8) are parallelograms. Since the faces normal to the shorter lattice vectors tend to be of greater area it is apparent that in this sense the Delaunay cell may ignore more than half of the total surface area of the Voronoi domain, and utilize vectors normal to tiny facets of that domain.

Mathematical proofs are collected in an Appendix.

2. The 'three shortest translations' and the Dirichlet reduced cell

Three lattice translations (**a**, **b**, **c**) are called 'three shortest non-coplanar translations' if

- **a** is the shortest vector in the lattice,
- **b** is the shortest vector other than $\pm\mathbf{a}$,
- **c** is the shortest vector not in the plane of **a** and **b**.

Such a triplet will form the edges of a primitive cell (Dirichlet, 1850) and have the properties

$$|\,\mathbf{a}\,| \le |\,\mathbf{b}\,| \le |\,\mathbf{c}\,|\,, \tag{2·1}$$

$$|\,\mathbf{b}\,| \le |\,\mathbf{b} \pm \mathbf{a}\,|\,, \tag{2·2}$$

$$|\,\mathbf{c}\,| \le |\,\mathbf{c} \pm \mathbf{a}\,|\,, \tag{2·3}$$

$$|\,\mathbf{c}\,| \le |\,\mathbf{c} \pm \mathbf{b}\,|\,, \tag{2·4}$$

$$|\,\mathbf{c}\,| \le |\,\mathbf{c} \pm \mathbf{a} \pm \mathbf{b}\,|\,. \tag{2·5}$$

It is obvious that these are necessary conditions for three shortest translations; together with the condition that (**a**, **b**, **c**) is a primitive triplet, they are also sufficient. In fact it follows from (2·1)–(2·5) that, for any integers (u, v, w),

$$|u\mathbf{a}+v\mathbf{b}+w\mathbf{c}| \geq |\mathbf{c}| \text{ unless } w = 0\,, \tag{2·6}$$

$$|u\mathbf{a}+v\mathbf{b}| \geq |\mathbf{b}| \text{ unless } v = 0\,. \tag{2·7}$$

These results we shall prove in the Appendix. From them we get

$$|u\mathbf{a}+v\mathbf{b}+w\mathbf{c}| \geq |\mathbf{b}| \text{ unless } v = w = 0\,, \tag{2·8}$$

$$|u\mathbf{a}+v\mathbf{b}+w\mathbf{c}| \geq |\mathbf{a}| \text{ unless } u = v = w = 0\,, \tag{2·9}$$

using (2·1) again; and from these results the sufficiency of the conditions will follow easily.

The conditions (2·1)–(2·5) ensure that (**a**, **b**, **c**) are 'three shortest translations'; the same conditions, but with strict inequality throughout, ensure that they are 'the three shortest translations', i.e. that they are unique apart from sign.

Observe that, given a primitive triplet which does not satisfy all the conditions (2·1)–(2·5), the particular condition which fails tells us precisely how to improve the triplet. This is applied in the reduction process in § 3.

The *Dirichlet reduced cell* is a parallelepiped having three shortest translations $\pm\mathbf{a}$, $\pm\mathbf{b}$, $\pm\mathbf{c}$ as its edges.

For Dirichlet's purpose the ambiguities of sign were quite irrelevant; and although he adopted an order convention equivalent to (2·1), this convention was self-evident in his applications. The crystallographer, however, needs to distinguish the direction [110] from the directions [1$\bar{1}$0], etc.

For order-convention we propose (2·1). The convenience of this has been pointed out by Balashov (1956) and, in the work of Dirichlet, it has by far the oldest tradition. Recent practice among crystallographers shows no uniform acceptance of any other convention: Buerger (1942, p. 346) advocates (2·1).

Suppose that the plane angles meeting at one corner of a parallelepiped are α, β, γ. The corner at the other end of the body-diagonal also gives angles (α, β, γ), while of the other six corners two give $(\alpha, \beta', \gamma')$, two give $(\alpha', \beta, \gamma')$ and two give $(\alpha', \beta', \gamma)$, where

$$\alpha' = \pi-\alpha,\ \beta' = \pi-\beta,\ \gamma' = \pi-\gamma\,.$$

For the general parallelepiped, for which α, β, γ are all distinct from 90°, there are just two corners at which the three angles are *homogeneous*, i.e. either all acute or all obtuse. In the first case we speak of an acute parallelepiped, in the second case of an obtuse one. We take one of the two homogeneous corners of the Dirichlet cell, and take the vectors **a**, **b**, **c** drawn from this corner along the edges meeting there.

To the change from one homogeneous corner to the other one (which is at the other end of the body-diagonal) corresponds a simultaneous change in sign of **a**, **b** and **c**. Thus if the one gives a right-handed frame (**a**, **b**, **c**), the other gives a left-handed frame. Following the usual crystallographic convention, we choose the right-handed one. This completes our rule of signs.

We may also express the rule as follows:

$$\mathbf{a}, \mathbf{b}, \mathbf{c} \text{ form a right-handed frame,} \tag{2·10}$$

$$\mathbf{b}.\mathbf{c},\ \mathbf{c}.\mathbf{a},\ \mathbf{a}.\mathbf{b} \text{ have the same sign,} \tag{2·11}$$

this last being equivalent to

$$\alpha, \beta, \gamma \text{ are all acute or all obtuse.} \tag{2·12}$$

If we have found a triplet (**a**, **b**, **c**) satisfying the conditions (2·1)–(2·10), and *not* satisfying (2·11), the three scalar products must include two of one sign and one of the opposite sign. If **b**.**c** is the 'odd man out' or, in terms of the angles, if α is the odd man out (if, for example, α is acute and β, γ both obtuse), then we reverse the signs of both **b** and **c** (so that α, β, γ become all acute).

Note that in producing homogeneity it is the two that have to come into step with the one: the product

$$(\mathbf{b}.\mathbf{c})\ (\mathbf{c}.\mathbf{a})\ (\mathbf{a}.\mathbf{b})$$

is positive for an acute parallelepiped, negative for an obtuse one, and its sign cannot be altered by any changes of sign of the three vectors. Note further that, in the case cited, homogeneity could be produced either by changing the sign of **a**, or by changing the signs of both **b** and **c**: we must choose the latter method in order to keep the frame right-handed.

To conclude this Section, we would like to mention that in a certain sense the Dirichlet triplet is the *most compact* triplet in the lattice. To bring out what we mean by this we observe first that when **a** has been chosen, the field of choice for **b** is restricted, and that when **b** has also been chosen, the field of choice for **c** is still further restricted. It is logically conceivable, therefore, that the choice of the shortest available **a** might force us to take an unduly long **c**. In our problem, however, this cannot occur. Instead of Dirichlet's rule, we could work from the other end. We could examine all primitive triplets (**a**, **b**, **c**), ordered by (2·1), and take only those for which **c**, the longest vector, was as short as possible. From these triplets we could pick out those for which **b** was as short as (now) possible; and finally pick out a triplet, from those still left, for which **a** was as short as possible. It would be natural to call a triplet obtained in this way the most compact. But in fact we get in this way exactly the same triplet or triplets as by Dirichlet's rule.

After this remark it becomes natural to ask whether the Dirichlet *cell* is not the most compact, in other words, whether there is another primitive parallelepiped whose diameter (i.e. longest body-diagonal) is shorter than the diameter of the Dirichlet cell. Very often the Dirichlet cell is the most compact, but not always: for example, the cell corresponding (cf. § 3) to the matrix

$$\begin{pmatrix} 20 & 9 & 9 \\ 9 & 22 & 5 \\ 9 & 5 & 24 \end{pmatrix}$$

is in fact a Dirichlet reduced cell of diameter $\sqrt{112}$, but the cell of edges $\mathbf{a}-\mathbf{b}$, $\mathbf{b}$, $\mathbf{c}$ has diameter only $\sqrt{98}$. The margin is never substantial.

3. The process of reduction

Suppose that we have a primitive triplet $(\mathbf{a}_0, \mathbf{b}_0, \mathbf{c}_0)$. We represent the geometry of this triplet by the symmetric matrix*

$$\mathbf{M}_0 = \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \\ \mathbf{c}_0 \end{pmatrix} . (\mathbf{a}_0 \; \mathbf{b}_0 \; \mathbf{c}_0)$$

$$= \begin{pmatrix} \mathbf{a}_0.\mathbf{a}_0 & \mathbf{a}_0.\mathbf{b}_0 & \mathbf{a}_0.\mathbf{c}_0 \\ \mathbf{b}_0.\mathbf{a}_0 & \mathbf{b}_0.\mathbf{b}_0 & \mathbf{b}_0.\mathbf{c}_0 \\ \mathbf{c}_0.\mathbf{a}_0 & \mathbf{c}_0.\mathbf{b}_0 & \mathbf{c}_0.\mathbf{c}_0 \end{pmatrix} = \begin{pmatrix} A_0 & H_0 & G_0 \\ H_0 & B_0 & F_0 \\ G_0 & F_0 & C_0 \end{pmatrix}, \quad (3{\cdot}1)$$

say. Here $A_0 = |\mathbf{a}_0|^2$ is the square of the length of $\mathbf{a}_0$, while $H_0 = \mathbf{a}_0.\mathbf{b}_0 = |\mathbf{a}_0|.|\mathbf{b}_0|.\cos\gamma_0$, where γ_0 is the angle between $\mathbf{a}_0$ and $\mathbf{b}_0$.

We first seek to improve, i.e. shorten, $\mathbf{b}_0$, $\mathbf{c}_0$ by adding to them multiples of $\pm\mathbf{a}_0$. In fact we replace $\mathbf{b}_0$, $\mathbf{c}_0$ by

$$\mathbf{b}_1 = \mathbf{b}_0 + m\mathbf{a}_0, \quad \mathbf{c}_1 = \mathbf{c}_0 + n\mathbf{a}_0,$$

where m is the integer nearest to $-H_0/A_0$ and n is the integer nearest to $-G_0/A_0$. Thus our first transformation is

$$\begin{pmatrix} \mathbf{a}_1 \\ \mathbf{b}_1 \\ \mathbf{c}_1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ m & 1 & 0 \\ n & 0 & 1 \end{pmatrix} . \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \\ \mathbf{c}_0 \end{pmatrix} \quad (3{\cdot}2)$$

and therefore also (by transposing)

$$(\mathbf{a}_1, \mathbf{b}_1, \mathbf{c}_1) = (\mathbf{a}_0, \mathbf{b}_0, \mathbf{c}_0) . \begin{pmatrix} 1 & m & n \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (3{\cdot}3)$$

Notice that the row $(1, m, n)$ in the last matrix is obtained from the row (A_0, H_0, G_0) of $\mathbf{M}_0$ by (i) reversing the signs of the non-diagonal elements, (ii) dividing through by the diagonal element, (iii) taking the nearest integers.

The new triplet $(\mathbf{a}_1, \mathbf{b}_1, \mathbf{c}_1)$ gives a new symmetric matrix

$$\mathbf{M}_1 = \begin{pmatrix} A_1 & H_1 & G_1 \\ H_1 & B_1 & F_1 \\ G_1 & F_1 & C_1 \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{b}_1 \\ \mathbf{c}_1 \end{pmatrix} . (\mathbf{a}_1, \mathbf{b}_1, \mathbf{c}_1)$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ m & 1 & 0 \\ n & 0 & 1 \end{pmatrix} . \mathbf{M}_0 . \begin{pmatrix} 1 & m & n \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (3{\cdot}4)$$

We next seek to shorten $\mathbf{a}_1$, $\mathbf{c}_1$ by adding to them multiples of $\mathbf{b}_1$. In fact we replace them by

$$\mathbf{a}_2 = \mathbf{a}_1 + l'\mathbf{b}_1, \quad \mathbf{c}_2 = \mathbf{c}_1 + n'\mathbf{b}_1,$$

where l' is the integer nearest to $-H_1/B_1$ and n' is the integer nearest to $-F_1/B_1$. And the geometry of the new triplet $(\mathbf{a}_2, \mathbf{b}_2, \mathbf{c}_2)$, in which of course $\mathbf{b}_2 = \mathbf{b}_1$, is given by the matrix

$$\mathbf{M}_2 = \begin{pmatrix} A_2 & H_2 & G_2 \\ H_2 & B_2 & F_2 \\ G_2 & F_2 & C_2 \end{pmatrix} = \begin{pmatrix} 1 & l' & 0 \\ 0 & 1 & 0 \\ 0 & n' & 1 \end{pmatrix} . \mathbf{M}_1 . \begin{pmatrix} 1 & 0 & 0 \\ l' & 1 & n' \\ 0 & 0 & 1 \end{pmatrix}. \quad (3{\cdot}5)$$

Then we try to shorten $\mathbf{a}_2$, $\mathbf{b}_2$, replacing them by

$$\mathbf{a}_3 = \mathbf{a}_2 + l''\mathbf{c}_2, \quad \mathbf{b}_3 = \mathbf{b}_2 + m''\mathbf{c}_2,$$

where l'' is the integer nearest to $-G_2/C_2$ and m'' is the integer nearest to $-F_2/C_2$: and we get a formula similar to (3·4), (3·5) for the new matrix $\mathbf{M}_3$.

These operations, which may be performed in any order, are in principle to be repeated until they produce no further change; we have then found a primitive triplet $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ for whose matrix $\mathbf{M}$

$$\left.\begin{aligned} |2F| \le B, \quad |2G| \le A, \quad |2H| \le A, \\ |2F| \le C, \quad |2G| \le C, \quad |2H| \le B. \end{aligned}\right\} \quad (3{\cdot}6)$$

If (2·1) happens to hold, i.e. if

$$A \le B \le C, \quad (3{\cdot}7)$$

then the second row of (3·6) follows from the first, while the first row expresses the conditions (2·2), (2·3), (2·4) on the face-diagonals of the cell. We have only, therefore, to check on (2·5), i.e. to see whether one of the four body-diagonals is shorter than $\mathbf{c}$. For the body-diagonal

$$\mathbf{c}' = \mu\mathbf{a} + \lambda\mathbf{b} + \mathbf{c}, \quad (3{\cdot}8)$$

where $\lambda = \pm 1$, $\mu = \pm 1$, we have

$$|\mathbf{c}'|^2 - C = A + B + 2\lambda F + 2\mu G + 2\lambda\mu H. \quad (3{\cdot}9)$$

If any one of the last three terms in (3·9) is positive, the whole expression is positive, by (3·6). Thus (2·5) is already satisfied unless both $FGH < 0$ and

$$A + B < |2F| + |2G| + |2H|, \quad (3{\cdot}10)$$

in which case we must apply the transformation (3·8), giving λ the sign opposite to that of F and μ the sign opposite to that of G.

If (3·7) does not hold, we proceed analogously. In all cases this gives the Dirichlet cell; and we conclude

* Only the elements of matrix theory are needed in what follows; but these are essential. The reader unfamiliar with them will find all that he needs for the present purpose in a book by Aitken (1939).

Table 1. *Example*

$$
\begin{array}{cccc}
\mathbf{T} & \mathbf{M} & \mathbf{T}' & \mathbf{N} \\
\begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} &
\begin{pmatrix} 48{\cdot}3 & 32{\cdot}9 & -31{\cdot}1 \\ 32{\cdot}9 & 26{\cdot}4 & -21{\cdot}1 \\ -31{\cdot}1 & -21{\cdot}1 & 20{\cdot}8 \end{pmatrix} &
\begin{pmatrix} 1 & -1 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} &
\begin{pmatrix} 48{\cdot}3 & -15{\cdot}4 & 17{\cdot}2 \\ 32{\cdot}9 & -6{\cdot}5 & 11{\cdot}8 \\ -31{\cdot}1 & 10{\cdot}0 & -10{\cdot}3 \end{pmatrix} \\
\begin{pmatrix} 1 & 0 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix} &
\begin{pmatrix} 48{\cdot}3 & -15{\cdot}4 & 17{\cdot}2 \\ -15{\cdot}4 & 8{\cdot}9 & -5{\cdot}4 \\ 17{\cdot}2 & -5{\cdot}4 & 6{\cdot}9 \end{pmatrix} &
\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -2 & 1 & 1 \end{pmatrix} &
\begin{pmatrix} 13{\cdot}9 & 1{\cdot}8 & 17{\cdot}2 \\ -4{\cdot}6 & 3{\cdot}5 & -5{\cdot}4 \\ 3{\cdot}4 & 1{\cdot}5 & 6{\cdot}9 \end{pmatrix} \\
\begin{pmatrix} 1 & 1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} &
\begin{pmatrix} 7{\cdot}1 & -1{\cdot}2 & 3{\cdot}4 \\ -1{\cdot}2 & 5{\cdot}0 & 1{\cdot}5 \\ 3{\cdot}4 & 1{\cdot}5 & 6{\cdot}9 \end{pmatrix} &
\begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} &
\begin{pmatrix} 2{\cdot}5 & -1{\cdot}2 & 3{\cdot}4 \\ 2{\cdot}3 & 5{\cdot}0 & 1{\cdot}5 \\ -2{\cdot}0 & 1{\cdot}5 & 6{\cdot}9 \end{pmatrix} \\
\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} &
\begin{pmatrix} 6{\cdot}8 & 2{\cdot}3 & -2{\cdot}0 \\ 2{\cdot}3 & 5{\cdot}0 & 1{\cdot}5 \\ -2{\cdot}0 & 1{\cdot}5 & 6{\cdot}9 \end{pmatrix} &
\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} &
\begin{pmatrix} -2{\cdot}3 & 6{\cdot}8 & -2{\cdot}0 \\ -5{\cdot}0 & 2{\cdot}3 & 1{\cdot}5 \\ -1{\cdot}5 & -2{\cdot}0 & 6{\cdot}9 \end{pmatrix} \\
 &
\begin{pmatrix} 5{\cdot}0 & -2{\cdot}3 & -1{\cdot}5 \\ -2{\cdot}3 & 6{\cdot}8 & -2{\cdot}0 \\ -1{\cdot}5 & -2{\cdot}0 & 6{\cdot}9 \end{pmatrix} & &
\end{array}
$$

$$
\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \\ \mathbf{c}_0 \end{pmatrix}
$$

$$
= \begin{pmatrix} 0 & -1 & 0 \\ 1 & 1 & -1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & -2 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \\ \mathbf{c}_0 \end{pmatrix} = \begin{pmatrix} 0 & -1 & -1 \\ -2 & 1 & -2 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \\ \mathbf{c}_0 \end{pmatrix}.
$$

$$
\mathbf{a} = -\mathbf{b}_0-\mathbf{c}_0, \quad \mathbf{b} = -2\mathbf{a}_0+\mathbf{b}_0-2\mathbf{c}_0, \quad \mathbf{c} = \mathbf{a}_0+\mathbf{c}_0
$$

by applying the order-convention and rule of signs to it.

In the worked example (Table 1), the first matrix of the column headed $\mathbf{M}$ is $\mathbf{M}_0$, and represents the initial information. It is the first to be written down.

We then *choose* to transform as in (3·2), using $\mathbf{a}_0$ to improve $\mathbf{b}_0$ and $\mathbf{c}_0$; we could instead have used $\mathbf{b}_0$ to improve $\mathbf{c}_0$ and $\mathbf{a}_0$, as in (3·5), or $\mathbf{c}_0$ to improve $\mathbf{a}_0$ and $\mathbf{b}_0$. The transforming matrices are $\mathbf{T}_0$ and its transpose $\mathbf{T}_0'$. When these have been entered we calculate

$$\mathbf{N}_0 = \mathbf{M}_0\mathbf{T}_0'$$

and use it to evaluate

$$\mathbf{M}_1 = \mathbf{T}_0\mathbf{M}_0\mathbf{T}_0' = \mathbf{T}_0\mathbf{N}_0\,,$$

which we write down underneath $\mathbf{M}_0$, ready for further reduction. At the next stage we could centre our transformation on the diagonal element $B = 8{\cdot}9$, as in (3·5); we *choose* instead to use $\mathbf{c}_1$ to improve $\mathbf{a}_1$ and $\mathbf{b}_1$. We calculate $\mathbf{N}_1 = \mathbf{M}_1\mathbf{T}_1'$ and then $\mathbf{M}_2 = \mathbf{T}_1\mathbf{N}_1$. At this stage we find (3·6) already satisfied, but $FGH<0$ and (3·10) holds. (Here $B+C$ must replace $A+B$, since A is the greatest.) Hence we transform as in (3·8); but since $\mathbf{a}_2$, not $\mathbf{c}_2$, is the longest, it is $\mathbf{a}_2$ that we replace, and by

$$\mathbf{a}_3 = \mathbf{a}_2+\nu\mathbf{b}_2+\mu\mathbf{c}_2 = \mathbf{a}_2+\mathbf{b}_2-\mathbf{c}_2\,,$$

where $\nu = \lambda\mu$ has the opposite sign to H. Notice that in this step $\mathbf{T}$ has a row, and therefore $\mathbf{T}'$ has a column, with non-diagonal elements different from zero, whereas in the previous steps it was the other way about. Notice also that these non-diagonal elements of $\mathbf{T}_2$ have signs opposite to those of the corresponding elements $(-1{\cdot}2,\ +3{\cdot}4)$ of $\mathbf{M}_2$.

The step from $\mathbf{M}_3$ to $\mathbf{M}_4$ secures simultaneously the order-convention and the rule of signs. The rows and columns are rearranged to satisfy (2·1), and the non-diagonal elements, if not already of the same sign, are given the sign of the 'odd man out'. In our example, G_3 is 'odd man out', and after the rearrangement $H_4 = -H_3$, $G_4 = -F_3$, $F_4 = +G_3$.

Some skill (or luck) is needed to write down at once the appropriate transforming matrix ($\mathbf{T}_3$) for this step: it should have determinant $+1$ in order that the final frame be right-handed. It is required only in order to give, with the correct signs, the relation between the initial and final triplets: this is in our case

$$\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix} = \mathbf{T}_3\mathbf{T}_2\mathbf{T}_1\mathbf{T}_0 . \begin{pmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \\ \mathbf{c}_0 \end{pmatrix},$$

and this is computed in the last part of our worked example.

4. From Delaunay cell to Dirichlet cell*

If Delaunay's algorism has been used, it gives a quartet (1·1) of lattice translations satisfying (1·2) and for which the Selling parameters (1·3) have been computed and are all negative. In the matrix

$$\mathbf{M}^* = \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \\ \mathbf{d} \end{pmatrix} . (\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}) = \begin{pmatrix} A & H & G & U \\ H & B & F & V \\ G & F & C & W \\ U & V & W & D \end{pmatrix}, \qquad (4{\cdot}1)$$

* In a very recent paper, Patterson & Love (1957) also give rules for obtaining the Dirichlet cell from the Delaunay one. Their rules would be equivalent to ours but for an unfortunate error by which all three conditions in their Table 1 have been stated with the inequalities reversed.

F, G, H, U, V, W are the Selling parameters and have therefore been computed, while A, B, C, D are given by the relations

$$A+H+G+U = 0, \ldots, \ldots, \ldots, \tag{4·2}$$

(i.e. each row of $\mathbf{M}^*$ adds up to zero), cf. (1·4). A, B, C, D also have been computed, first in order to discard the longest of the quartet, say $\mathbf{d}$, and then in order to calculate the edge-lengths

$$a = \sqrt{A}, \quad b = \sqrt{B}, \quad c = \sqrt{C}$$

and angles

$$\alpha = \cos^{-1}(F/bc), \ldots, \ldots,$$

of the 'Delaunay reduced cell', cf. (1·5). We may therefore suppose $\mathbf{M}^*$ already computed, and it is at this point that we interrupt the work leading to the Delaunay cell.

To fix the ideas, suppose that

$$A < B < C < D. \tag{4·3}$$

There are four cases:

(i) If $A+2H < 0$ we replace $\mathbf{b}$ by $\mathbf{b}' = \mathbf{a}+\mathbf{b}$, retaining $\mathbf{a}$ and $\mathbf{c}$. The triplet $(\mathbf{a}, \mathbf{b}', \mathbf{c})$ gives a matrix

$$\mathbf{M}' = \begin{pmatrix} A & A+H & G \\ A+H & A+2H+B & F+G \\ G & F+G & C \end{pmatrix}.$$

(ii) If $A+2G < 0$ we replace $\mathbf{c}$ by $\mathbf{c}' = \mathbf{a}+\mathbf{c}$. The triplet $(\mathbf{a}, \mathbf{b}, \mathbf{c}')$ gives

$$\mathbf{M}' = \begin{pmatrix} A & H & A+G \\ H & B & F+H \\ A+G & F+H & A+2G+C \end{pmatrix}.$$

(iii) If $B+2F < 0$ we replace $\mathbf{c}$ by $\mathbf{c}' = \mathbf{b}+\mathbf{c}$, and the triplet $(\mathbf{a}, \mathbf{b}, \mathbf{c}')$ gives

$$\mathbf{M}' = \begin{pmatrix} A & H & G+H \\ H & B & B+F \\ G+H & B+F & B+2F+C \end{pmatrix}.$$

(The cases (i), (ii), (iii) do not overlap. For it may be shown, using (4·2) and (4·3), that the sum of any two of the three quantities $A+2H$, $A+2G$, $B+2F$ is positive.)

(iv) In the remaining cases the Delaunay cell is the Dirichlet one.

In the first three cases three simple additions give the new matrix elements in $\mathbf{M}'$, and the triplets stated give the Dirichlet cell. In each case we have still to make them satisfy our order-convention and rule of signs.

Finally, if we wish to present the results in the form $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, (α, β, γ), then we have to calculate one new length and two new angles, and also, possibly, replace the third angle by its supplement.

Table 2. *Illustrations*

In each of the following seven illustrations, the first row gives the dimensions of the experimental cell, the second row gives those of the Dirichlet reduced cell and the third row gives those of the Delaunay reduced cell (but with (2·1) as order-convention)

	a (Å)	b (Å)	c (Å)	α	β	γ
1	9·029	11·56	5·52	103° 49′	101° 45′	87° 12′
	5·52	9·029	11·56	87° 12′	76° 11′	78° 15′
	9·029	9·575	11·56	95° 48′	92° 48′	145° 39′
2	15·10	8·80	7·25	95° 23′	92° 37′	88° 58½′
	7·25	8·80	15·10	88° 58½′	87° 23′	84° 37′
	8·80	10·86	15·10	90° 55′	91° 1½′	138° 22′
3	15·25	8·97	7·25	95° 00′	92° 18′	89° 23′
	7·25	8·97	15·25	89° 23′	87° 42′	85°
	8·97	11·03	15·25	91° 1′	90° 37′	139° 6′
4	5·30	8·61	16·20	103°	107°	98°
	5·30	8·61	15·46	74° 8′	87° 39′	82°
	5·30	9·46	15·46	103° 3′	92° 21′	115° 42′
5	4·653	4·097	35·33	103° 51′	95° 59′	77° 53′
	4·097	4·653	34·30	86° 43′	89° 34′	77° 53′
	4·097	5·517	34·30	92° 26′	90° 26′	124° 27′
6	4·588	4·016	20·41	101° 12′	102° 28′	80° 04′
	4·016	4·588	19·69	87° 28′	87° 33′	80° 04′
	4·016	4·588	19·93	90° 31′	99° 9′	99° 56′
7	16·9	15·8	6·9	98°	95°	89°
	6·9	15·8	16·9	89°	85°	82°
	15·8	16·34	16·9	91° 8′	91°	155°

1: Yeatmanite, $(Mn, Zn)_{16}Sb_2Si_4O_{29}$ (Palache, Bauer & Berman, 1938).
2: Diammonium nickel cyanide trihydrate,

$(NH_4)_2Ni(CN)_4 3\,H_2O$

(Brasseur & de Rassenfosse, 1941).
3: Disodium platinum cyanide trihydrate, $Na_2Pt(CN)_4 3\,H_2O$ (Brasseur & de Rassenfosse, 1941).
4: DL-Tryptophane dihydrochloride, $C_{11}H_{12}N_2O_2 . 2\,HCl$ (Dawson & Mathieson, 1951).
5: Silver laurate, $C_{11}H_{23}COOAg$ (Vand, Aitken & Campbell, 1949).
6: Silver caproate, $C_5H_{11}COOAg$ (Vand, Aitken & Campbell, 1949).
7: Methylene blue iodide trihydrate $C_{16}H_{18}N_3SI . 3\,H_2O$ (Taylor, 1935).

The experimental data published for 136 triclinic crystals show that
for 85 the experimental cell is the Dirichlet cell,
for 39 the Dirichlet cell requires one change in the edges of the experimental cell, and
for 12 two changes are required.

The corresponding figures for the Delaunay reduced cell are 50, 66, 20.

APPENDIX

1. Suppose that a primitive triplet $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ satisfies conditions (2·1)–(2·5). Then the elements in the corresponding matrix $\mathbf{M}$ satisfy

$$A \leq B \leq C, \tag{A1}$$

$$|2F| \leq B, \quad |2G| \leq A, \quad |2H| \leq A, \tag{A2}$$

(These express (2·1)–(2·4), but leave (2·5) unexpressed.) Our first object is to deduce (2·6). Write

$$u' = |u|, \quad v' = |v|, \quad w' = |w| .$$

Then

$$\begin{aligned} &u'^2+v'^2+w'^2-v'w'-w'u'-u'v' \\ &= \tfrac{1}{2}(v'-w')^2+\tfrac{1}{2}(w'-u')^2+\tfrac{1}{2}(u'-v')^2 \\ &> 0 \text{ unless } u' = v' = w' . \end{aligned} \quad \text{(A3)}$$

Hence, also,

$$v'^2+w'^2-v'w' > 0 \text{ unless } v' = w' = 0 .$$

Since these expressions are certainly integers, > 0 means the same as ≥ 1. Now suppose $w \neq 0$ and so $w' \geq 1$. Then *unless* $u' = v' = w'$,

$$\begin{aligned} |u\mathbf{a}+v\mathbf{b}+w\mathbf{c}|^2 &= Au^2+Bv^2+Cw^2+2Fvw+2Gwu+2Huv \\ &\geq Au'^2+Bv'^2 \\ &\quad +Cw'^2-Bv'w'-Aw'u'-Au'v' \\ &= A(u'^2+v'^2+w'^2-v'w'-w'u'-u'v') \\ &\quad +(B-A)(v'^2+w'^2-v'w')+(C-B)w'^2 \\ &\geq A+(B-A)+(C-B) = C , \end{aligned} \quad \text{(A4)}$$

$$|u\mathbf{a}+v\mathbf{b}+w\mathbf{c}| \geq |\mathbf{c}| .$$

If, on the other hand, $u' = v' = w'$,

$$|u\mathbf{a}+v\mathbf{b}+w\mathbf{c}| = w'|\mathbf{c}\pm\mathbf{a}\pm\mathbf{b}| \geq |\mathbf{c}| ,$$

by (2·5). This proves (2·6); the proof of (2·7) is similar, and (2·8), (2·9) are obvious consequences.

2. To see that (2·1)–(2·5) are sufficient conditions, let $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ be *any* three non-coplanar vectors belonging to the lattice. Then one at least of the three must be at least as long as $\mathbf{c}$, since by (2·6) all lattice vectors shorter than $\mathbf{c}$ must lie in the plane of $\mathbf{a}$ and $\mathbf{b}$. By (2·8), at least two of the three must be at least as long as $\mathbf{b}$, and by (2·9) each of them must be at least as long as $\mathbf{a}$. Thus if we order the three so that

$$|\mathbf{a}'| \leq |\mathbf{b}'| \leq |\mathbf{c}'| ,$$

we shall have

$$|\mathbf{a}'| \geq |\mathbf{a}|, \quad |\mathbf{b}'| \geq |\mathbf{b}|, \quad |\mathbf{c}'| \geq |\mathbf{c}| . \quad \text{(A5)}$$

(A5) shows that $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ are three shortest translations, i.e. the conditions are sufficient, and at the same time shows that $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is a 'most compact' triplet of independent translations. It is to be noted that in proving (A5) we have not assumed that $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ is a *primitive* triplet.

3. As to uniqueness of the three shortest translations, this obviously requires strict inequality throughout (2·1)–(2·5). To prove that strict inequality throughout is sufficient for uniqueness we first sharpen (2·6) to the result that

$$|u\mathbf{a}+v\mathbf{b}+w\mathbf{c}| > |\mathbf{c}| \quad \text{(A6)}$$

unless either $w = 0$ or $u = v = 0$ and $w = \pm 1$.

Now if $u' = v' = w'$, (A6) is given by (2·5), in which, by hypothesis, strict inequality now reigns. In any other case in which $w \neq 0$, equality in (2·6) requires equality throughout in (A4). Equality in the first step requires

$$v'w' = w'u' = u'v' = 0 ,$$

since strict inequality now holds in (A2); and equality in the last step of (A4) requires $w' = 1$. This proves (A6), with the exceptions stated.

For a triplet $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ to be as compact as $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, i.e. to give equality in (A5), it is therefore necessary that $\mathbf{c}' = \pm\mathbf{c}$ and that $\mathbf{a}', \mathbf{b}'$ be in the plane of $\mathbf{a}$ and $\mathbf{b}$. We may similarly sharpen (2·7) and so show that $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ are unique, apart from their signs, either as three shortest translations or as most compact triplet.

If (2·1)–(2·5) hold, but not with strict inequality, then it may be shown that an alternative set $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$, either as three shortest translations or as most compact triplet, must be made up of three of the thirteen vectors

$$\mathbf{a}, \mathbf{b}, \mathbf{c}, \ \mathbf{b}\pm\mathbf{c}, \ \mathbf{c}\pm\mathbf{a}, \ \mathbf{a}\pm\mathbf{b}, \ \mathbf{c}\pm\mathbf{a}\pm\mathbf{b}$$

which appear in (2·1)–(2·5).

4. We shall justify the transformation applied in case (i) of § 4. In that case we had

$$A+2H < 0, \quad A < B < C < D ,$$

and proposed the triplet $(\mathbf{a}, \mathbf{b}', \mathbf{c})$, where $\mathbf{b}' = \mathbf{a}+\mathbf{b}$. For the corresponding matrix $\mathbf{M}'$,

$$\begin{aligned} &A' = A, \ B' = A+2H+B, \ C' = C , \\ &F' = F+G, \ G' = G, \ H' = A+H, \\ &F' < 0, \ G' < 0, \ H' > 0, \\ &B'+2F' = D-C > 0, \\ &|2F'| = -2F' < B' < B < C = C', \\ &A+2G = -(A+2H)-2U > 0, \\ &|2G'| = -2G < A = A' < C = C', \\ &2H'-A' < 0, \ 2H'-B' < 0, \\ &|2H'| < A', \ |2H'| < B'. \end{aligned}$$

This shows that the new cell is an *acute* parallelepiped satisfying the face-diagonal conditions (3·6), and therefore also the body-diagonal conditions. It is therefore the Dirichlet cell, though we have still to apply the order-convention and rule of signs.

The transformations given for the other cases of § 4 are similarly justified.

5. To justify our statements about Voronoi domains we start from a Selling reduced quartet, as in § 4, but make no assumption (4·3) as to the relative magnitudes of $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$, and so shall have complete algebraic symmetry. The point $\mathbf{r} \doteq x\mathbf{a}+y\mathbf{b}+z\mathbf{c}$ is nearer to the origin than to the lattice point $\mathbf{e} = u\mathbf{a}+v\mathbf{b}+w\mathbf{c}$ if

$$\mathbf{r}.\mathbf{e} < \tfrac{1}{2}\mathbf{e}^2. \quad \text{(A7)}$$

The Voronoi domain about the origin is defined by all the inequalities (A7), in which $\mathbf{e}$ runs through all lattice points other than the origin. Now suppose that a point $\mathbf{r}$ satisfies

$$\mathbf{r}.\mathbf{e}' < \tfrac{1}{2}\mathbf{e}'^2 \tag{A8}$$

for each of the following 14 values of $\mathbf{e}'$:

$$\pm\mathbf{a},\ \pm\mathbf{b},\ \pm\mathbf{c},\ \pm\mathbf{d}\ , \tag{A9}$$

$$\pm(\mathbf{b}+\mathbf{c}),\ \pm(\mathbf{c}+\mathbf{a}),\ \pm(\mathbf{a}+\mathbf{b})\ . \tag{A10}$$

If

$$0 \le u \le v \le w\ , \tag{A11}$$

we write

$$\mathbf{e} = u(\mathbf{a}+\mathbf{b}+\mathbf{c})+(v-u)(\mathbf{b}+\mathbf{c})+(w-v)\mathbf{c} = u_1\mathbf{e}_1+u_2\mathbf{e}_2+u_3\mathbf{e}_3\ , \tag{A12}$$

say, where u_1, u_2, u_3 are non-negative integers, and $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are three of the 14 vectors $\mathbf{e}'$, and are *neighbours* in the sense that their scalar products are positive. Hence

$$\begin{aligned}\mathbf{r}.\mathbf{e} &= u_1\mathbf{r}.\mathbf{e}_1+u_2\mathbf{r}.\mathbf{e}_2+u_3\mathbf{r}.\mathbf{e}_3\\ &< \tfrac{1}{2}u_1\mathbf{e}_1^2+\tfrac{1}{2}u_2\mathbf{e}_2^2+\tfrac{1}{2}u_3\mathbf{e}_3^2\\ &\le \tfrac{1}{2}u_1^2\mathbf{e}_1^2+\tfrac{1}{2}u_2^2\mathbf{e}_2^2+\tfrac{1}{2}u_3^2\mathbf{e}_3^2\\ &\le \tfrac{1}{2}(u_1\mathbf{e}_1+u_2\mathbf{e}_2+u_3\mathbf{e}_3)^2 = \tfrac{1}{2}\mathbf{e}^2\ .\end{aligned}$$

If (A11) is not satisfied, but u, v, w are all non-negative, we apply the same argument with $\mathbf{a}, \mathbf{b}, \mathbf{c}$ suitably permuted. If one of u, v, w is negative, let u be the algebraically least; then express $\mathbf{e}$ in terms of $\mathbf{b}, \mathbf{c}, \mathbf{d}$ instead of $\mathbf{a}, \mathbf{b}, \mathbf{c}$, and argue as before.

Thus all the inequalities (A7) follow from the 14 inequalities (A8), and so the Voronoi domain has *at most* 14 faces

$$\mathbf{r}.\mathbf{e}' = \tfrac{1}{2}\mathbf{e}'^2\ . \tag{A13}$$

To see that the domain has in general all these faces, we consider the point given by three planes (A13) which are neighbours in the above sense, e.g. the above set

$$\mathbf{c},\ \mathbf{b}+\mathbf{c},\ \mathbf{a}+\mathbf{b}+\mathbf{c}\ (= -\mathbf{d})\ , \tag{A14}$$

and show that this point satisfies the other 11 inequalities (A8). We have, for instance,

$$\begin{aligned}\mathbf{r}.\mathbf{b} &= \mathbf{r}.(\mathbf{b}+\mathbf{c})-\mathbf{r}.\mathbf{c} = \tfrac{1}{2}(\mathbf{b}+\mathbf{c})^2-\tfrac{1}{2}\mathbf{c}^2 < \tfrac{1}{2}\mathbf{b}^2,\\ 2|\mathbf{r}.(\mathbf{a}+\mathbf{c})| &= |(\mathbf{a}+\mathbf{b}+\mathbf{c})^2-(\mathbf{b}+\mathbf{c})^2+\mathbf{c}^2|\\ &= |A+2H+2G+C| < A+2G+C=|\mathbf{a}+\mathbf{c}|^2\ .\end{aligned}$$

It follows that the 24 points obtained in this way by permuting $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ in (A14) are the corners of the domain, and so that it has indeed all the 14 planes (A13) as faces. The neighbours of $-\mathbf{d}$ form the cycle

$$\ldots,\ \mathbf{a},\ \mathbf{a}+\mathbf{b},\ \mathbf{b},\ \mathbf{b}+\mathbf{c},\ \mathbf{c},\ \mathbf{c}+\mathbf{a},\ \mathbf{a},\ \ldots$$

and so $\mathbf{e}' = -\mathbf{d}$ gives a six-sided face. The neighbours of $\mathbf{b}+\mathbf{c}$ form the cycle

$$\ldots,\ -\mathbf{a},\ \mathbf{b},\ -\mathbf{d},\ \mathbf{c},\ -\mathbf{a},\ \ldots$$

and so $\mathbf{e}' = \mathbf{b}+\mathbf{c}$ gives a four-sided face.

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