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# The Relationship between Reduced Cells in a General Bravais lattice

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*To my mother on the occasion of her* 81*st birthday*

It is shown that in a three-dimensional Bravais lattice at most 5 different cells based on the shortest three non-coplanar translations (Buerger cells) may exist. Their mutual relationship is found and two procedures are proposed to find all these cells if one of them is known. That cell which corresponds to the reduced quadratic form is indicated. For any of the 14 types of Bravais lattice the number of different Buerger cells is ascertained.

## Introduction

It has been noted by several authors that the Buerger cell, *i.e.* the cell based on the shortest three non-coplanar translations, is not unique in many cases and some particular ambiguities have been demonstrated (*e.g.* Santoro & Mighell, 1970). However, the general conditions under which these ambiguities can occur have not yet been found nor is it known how many different Buerger cells may exist in an arbitrary lattice. A general solution of this problem is given in the present paper. Assuming that one of the Buerger cells of a Bravais lattice is given, two different ways are proposed for ascertaining the number of different Buerger cells of this lattice and the relationship among them. Table 1 shows that there are lattices with 1, 2, 3, 4 or 5 different Buerger cells, but no lattice can have a greater number. Moreover the Table indicates which of the Buerger cells is the Niggli (1928) cell, *i.e.* the cell based on the reduction theory of the positive definite quadratic forms. It also contains the matrices by means of which any Buerger cell may be converted into the Niggli cell; this is an alternative to Santoro & Mighell's (1970) procedure. The significance of the Niggli cell is in its uniqueness and in the possibility that it can be used for determining the type of lattice. The application of the Niggli forms shows that the ambiguity of the Buerger cells is not an exceptional case since it occurs in 7 of the 14 types of Bravais lattice.

In addition it will be shown that the algorithm for determining the Buerger cell proposed by Buerger (1957, 1960) can be substantially quickened if the function *entier* is applied. As far as the terminology is concerned we avoid the term 'reduced cell' entirely since it has been used in different senses and could easily cause further misunderstanding.

## Buerger cell

For our purposes it is convenient to deviate from the usual matrix representation

$$\begin{pmatrix} S_{11} & S_{22} & S_{33} \\ S_{23} & S_{13} & S_{12} \end{pmatrix}$$

of a cell. Instead we shall use a sequence of six real numbers

$$A,\ B,\ C,\ \xi,\ \eta,\ \zeta \tag{1}$$

defined by

$$\begin{array}{lll} A=\mathbf{a}^2, & B=\mathbf{b}^2, & C=\mathbf{c}^2, \\ \xi=2\mathbf{b}\,.\,\mathbf{c}\,, & \eta=2\mathbf{a}\,.\,\mathbf{c}\,, & \zeta=2\mathbf{a}\,.\,\mathbf{b} \end{array} \tag{2}$$

so that

$$\begin{array}{lll} A=S_{11}\,, & B=S_{22}\,, & C=S_{33}\,, \\ \xi=2S_{23}\,, & \eta=2S_{13}\,, & \zeta=2S_{12}\,. \end{array}$$

The sequence (1) will be referred to as the characteristic of the cell in question. There are good reasons for this different notation. We shall need the double indices in other places and we also hope that the tables will be easier to survey, so that it will be possible to run through them more quickly.

We say that (1) is a characteristic of the lattice $L$, if it is a characteristic of a primitive cell of this lattice. We say that it is a Buerger characteristic of $L$, if it is a characteristic of a Buerger cell of $L$.

A cell may always be labelled in such a way that the following conditions are fulfilled:

1. $A\le B\le C$;
2. if $A=B$, then $|\xi|\le|\eta|$;
3. if $B=C$, then $|\eta|\le|\zeta|$;
4. it holds that either $\xi>0\,,\quad \eta>0\,,\quad \zeta>0\,,$
   or $\xi\le 0\,,\quad \eta\le 0\,,\quad \zeta\le 0\,.$ (3)

If this occurs the characteristic (1) is said to be normalized. We say that we normalize the characteristic of a cell $U$, if we change it (if necessary) by relabelling $U$ so that it becomes normalized. This may be done by means of this simple Algorithm $N$.

*Algorithm N*

$N1$. If $A>B$ or $A=B$, $|\xi|>|\eta|$, change $(A,\xi)\leftrightarrow(B,\eta)$.*

$N2$. If $B>C$ or $B=C$, $|\eta|>|\zeta|$, change $(B,\eta)\leftrightarrow(C,\zeta)$ and go to the point $N1$.

$N3$. If $\xi\eta\zeta>0$, put $|\xi|\to\xi$, $|\eta|\to\eta$, $|\zeta|\to\zeta$; otherwise put $-|\xi|\to\xi$, $-|\eta|\to\eta$, $-|\zeta|\to\zeta$.

* $N1$ is equivalent to the following Algol 60 statement: *begin if* $A>B\vee A=B\wedge \mathrm{abs}(\xi)>\mathrm{abs}(\eta)$ *then begin* $p:=A$; $A:=B$; $B:=p$; $p:=\xi$; $\xi:=\eta$; $\eta:=p$ *end end.*

The normalized characteristic of a cell is unique.

Whether a cell is a Buerger one or not can be ascertained by the following:

*Theorem* 1 (Buerger, 1960): Let (1) be the normalized characteristic of a primitive cell $U$. Then $U$ is a Buerger cell if and only if the following inequalities hold:

$$|\xi| \le B\,,\quad |\eta| \le A\,,\quad |\zeta| \le A$$
$$\xi+\eta+\zeta+A+B \ge 0\,. \qquad (4)$$

Gruber (1970) gave a more general criterion where the interaxial angles need not be all acute or all obtuse and the primitiveness of the cell is not assumed.

The starting point of our procedures will be a normalized Buerger characteristic of the lattice under investigation. It may be easily recognized since it must fulfil conditions (3) and (4) which are also sufficient. It can be obtained by means of the algorithm proposed by Buerger (1960). This algorithm is based on the fact that if two vectors **r**, **s** satisfy the inequalities

$$2|\mathbf{r}\,.\,\mathbf{s}| > \mathbf{r}^2 > 0\,,$$

then an integer $m$ can be found such that

$$2|\mathbf{r}\,.\,(\mathbf{s}-m\mathbf{r})| \le \mathbf{r}^2\,.$$

This integer $m$ is determined in the Buerger algorithm in a succesive way by subtracting the value $\mathbf{r}^2$ from the number $|\mathbf{r}\,.\,\mathbf{s}|$ so many times until the change of sign occurs. But $m$ may be picked out immediately by putting

$$m = \text{entier}\ (\mathbf{r}\,.\,\mathbf{s}/\mathbf{r}^2+\tfrac{1}{2})\,.$$

The function entier $x$ used in Algol 60 means the greatest integer which is not greater than $x$ ($0 \le x -$ entier $x < 1$). In this way the procedure may be quickened considerably when we start 'far' from the Buerger cell. For the convenience of the reader the complete algorithm is formulated here in our notation with all details so that it can be directly transcribed into a computer language.

*Theorem* 2. Let (1) be a characteristic of the lattice $L$, let us carry out Algorithm $B$. Then the sequence (1) with the new values is a normalized Buerger characteristic of the lattice $L$.

*Algorithm B*

$B1$. Carry out algorithm $N$.

$B2$. If $|\xi| > B$, put

$$\begin{array}{ll} \text{entier}\ ((\xi+B)/2B) & \to j\,,^* \\ C+j^2B-j\xi & \to C\,, \\ \xi-2jB & \to \xi\,, \\ \eta-j\zeta & \to \eta \end{array}$$

and go to the point $B1$.

$B3$. If $|\eta| > A$, put

$$\begin{array}{ll} \text{entier}\ ((\eta+A)/2A) & \to j\,,^\dagger \\ C+j^2A-j\eta & \to C\,, \\ \xi-j\zeta & \to \xi\,, \\ \eta-2jA & \to \eta \end{array}$$

and go to the point $B1$.

$B4$. If $|\zeta| > A$, put

$$\begin{array}{ll} \text{entier}\ ((\zeta+A)/2A) & \to j\,,^\ddagger \\ B+j^2A-j\zeta & \to B\,, \\ \xi-j\eta & \to \xi\,, \\ \zeta-2jA & \to \zeta \end{array}$$

and go to the point $B1$.

$B5$. If $\xi+\eta+\zeta+A+B<0$, put

$$\begin{array}{ll} \text{entier}\ (((\xi+\eta+\zeta+A+B)/2(A+B+\zeta))) & \to j\,,\S \\ C+j^2(A+B+\zeta)-j(\xi+\eta) & \to C\,, \\ \xi-j(2B+\zeta) & \to \xi\,, \\ \eta-j(2A+\zeta) & \to \eta \end{array}$$

and go to the point $B1$.

The use of the function sign instead of entier simplifies the calculation, but increases the number of steps.

### System of all Buerger cells

As has been already mentioned, the Buerger cell is in general not unique. The number of different Buerger cells in a lattice will be referred to as the index of this lattice. Since the normalized characteristics correspond in a unique way to the primitive cells, the index of a lattice is equal to the number of normalized Buerger characteristics of this lattice.

Our main task is to obtain all Buerger cells if one of them is known and to ascertain the relationship among them. In other words we want to find all normalized Buerger characteristics of the lattice if one such characteristic is given. Two ways are shown how to achieve this. The first is more 'theoretical' and yields a deeper insight into the problem. The second is rather 'numerical' and can be modified for a computer.

*Theorem* 3. Let (1) be a normalized Buerger characteristic of the lattice $L$, let the numbers $i_k$, conditions $C_k$, expressions $\xi_{km}$, $\eta_{km}$, $\zeta_{km}$ and matrices $\mathsf{M}_{kn}$ ($k=1,\ldots,28$; $m=1,\ldots,i_k$; $n=2,\ldots,i_k$) be given by Table 1, where $\mu=B/A$, $\nu=(B-A)/A$. Then the following is true:

($a$) If such integers $j$, $h$ ($1 \le j \le 28$; $1 \le h \le i_j$) and real numbers $p$, $q$ ($0<p<q\le A$) exist that the condition

* Or alternatively sign $\xi \to j$, where sign $x=1$ for $x>0$ and sign $x=\bar{1}$ for $x<0$.

† Or sign $\eta \to j$.

‡ Or sign $\zeta \to j$.

§ Or sign $(\xi+\eta) \to j$.

Table 1. *Relationships among Buerger cells*

| $k$ | $i_k$ | $C_k$ | $\xi_{k1}$ … $\xi_{kt_k}$ | $\eta_{k1}$ … $\eta_{kt_k}$ | $\zeta_{k1}$ … $\zeta_{kt_k}$ | $M_{k2}$ … $M_{kt_k}$ |
|---|---|---|---|---|---|---|
| 1 | 2 | $A=B\le C$ | $q$ | $q$ | $A$ | $N$ |
| | | or $A<B=C$ | $0$ | $-q$ | $-A$ | $100/110/00\bar{1}$ |
| 2 | 2 | $A=B\le C$ | $q/2$ | $q$ | $A$ | $N$ |
| | | | $-q/2$ | $-q/2$ | $-A$ | $110/010/00\bar{1}$ |
| 3 | 3 | $A=B\le C$ | $q-p/2$ | $q$ | $A$ | $N$ |
| | | | $p/2$ | $q$ | $A$ | $100/1\bar{1}0/001$ |
| | | | $-p/2$ | $-q+p/2$ | $-A$ | $110/100/00\bar{1}$ |
| 4 | 2 | $A\le B<C$ | $q$ | $A$ | $q$ | $N$ |
| | | | $0$ | $-A$ | $-q$ | $100/0\bar{1}0/101$ |
| 5 | 2 | $q<A=B<C$ | $q-p/2$ | $A$ | $q$ | $N$ |
| | | or $A<B<C$ | $p/2$ | $A$ | $q$ | $100/010/10\bar{1}$ |
| 6 | 2 | $A=B<C$ | $q$ | $A$ | $q/2$ | $N$ |
| | | | $-q/2$ | $-A$ | $-q/2$ | $100/0\bar{1}0/101$ |
| 7 | 2 | $A=B<C$ | $q$ | $A$ | $p/2$ | $N$ |
| | | | $-q+p/2$ | $-A$ | $-p/2$ | $100/0\bar{1}0/101$ |
| 8 | 2 | $A=B<C$ | $q$ | $A$ | $q-p/2$ | $N$ |
| | | | $-p/2$ | $-A$ | $-q+p/2$ | $100/0\bar{1}0/101$ |
| 9 | 2 | $A<B=C$ | $q-p/2$ | $q$ | $A$ | $N$ |
| | | or $q<A<B<C$ | $p/2$ | $q$ | $A$ | $100/1\bar{1}0/001$ |
| 10 | 2 | $A<B\le C$ | $B+\mu(p-q)$ | $p$ | $A$ | $N$ |
| | | | $-B-\nu p+\mu q$ | $-p$ | $-A$ | $100/110/00\bar{1}$ |
| 11 | 3 | $q=A<B=C$ | $B$ | $A$ | $q$ | $N$ |
| | | or $A<B<C$ | $-B$ | $-A+q$ | $-q$ | $100/0\bar{1}0/0\bar{1}\bar{1}$ |
| | | | $-B+q$ | $-A$ | $-q$ | $100/0\bar{1}0/101$ |
| 12 | 2 | $A<B=C$ | $\nu p+q$ | $q$ | $A$ | $N$ |
| | | | $-\nu p$ | $-q$ | $-A$ | $100/110/00\bar{1}$ |
| 13 | 3 | $A<B=C$ | $B$ | $A/2$ | $A$ | $N$ |
| | | | $-B$ | $-A/2$ | $-A/2$ | $100/0\bar{1}\bar{1}/00\bar{1}$ |
| | | | $-B+A/2$ | $-A/2$ | $-A$ | $100/110/00\bar{1}$ |
| 14 | 2 | $q<A<B=C$ | $B$ | $q$ | $q$ | $N$ |
| | | | $-B$ | $0$ | $-q$ | $100/0\bar{1}0/0\bar{1}\bar{1}$ |
| 15 | 2 | $q<A<B=C$ | $B$ | $q/2$ | $q$ | $N$ |
| | | | $-B$ | $-q/2$ | $-q/2$ | $100/0\bar{1}\bar{1}/00\bar{1}$ |
| 16 | 2 | $q<A<B=C$ | $-B+A-2q/3$ | $-A+q/3$ | $-A+q/3$ | $N$ |
| | | | $-B+q/3$ | $-2q/3$ | $-A+q/3$ | $100/010/\bar{1}\bar{1}\bar{1}$ |
| 17 | 2 | $q<A<B=C$ | $-B+A/2-q/6$ | $-A/2-q/6$ | $-A+q/3$ | $N$ |
| | | | $-B+q/3$ | $-A/2-q/6$ | $-A/2-q/6$ | $100/\bar{1}\bar{1}\bar{1}/001$ |
| 18 | 3 | $q<A<B=C$ | $B$ | $q-p/2$ | $q$ | $N$ |
| | | | $B$ | $p/2$ | $q$ | $100/010/01\bar{1}$ |
| | | | $-B$ | $-p/2$ | $-q+p/2$ | $100/0\bar{1}\bar{1}/0\bar{1}0$ |
| 19 | 3 | $q<A<B=C$ | $-B+A-p/6-q/2$ | $-A-p/6+q/2$ | $-A+p/3$ | $N$ |
| | | | $-B+p/3$ | $-p/6-q/2$ | $-A-p/6+q/2$ | $100/\bar{1}\bar{1}\bar{1}/010$ |
| | | | $-B-p/6+q/2$ | $-p/6-q/2$ | $-A+p/3$ | $100/010/\bar{1}\bar{1}\bar{1}$ |
| 20 | 5 | $q<A<B=C$ | $B$ | $A-q/2$ | $A$ | $N$ |
| | | | $B$ | $q/2$ | $A$ | $100/010/01\bar{1}$ |
| | | | $-B$ | $-q/2$ | $-A+q/2$ | $100/0\bar{1}\bar{1}/0\bar{1}0$ |
| | | | $-B+q/2$ | $-q/2$ | $-A$ | $100/110/111$ |
| | | | $-B+A-q/2$ | $-A+q/2$ | $-A$ | $100/110/00\bar{1}$ |
| 21 | 2 | $q<A<B<C$ | $B$ | $q-p/2$ | $q$ | $N$ |
| | | | $B$ | $p/2$ | $q$ | $100/010/01\bar{1}$ |
| 22 | 2 | $q<A<B<C$ | $-B+A+p/2-q$ | $-A+p/2$ | $-A-p+q$ | $N$ |
| | | | $-B+p/2$ | $-q+p/2$ | $-A-p+q$ | $100/010/\bar{1}\bar{1}\bar{1}$ |
| 23 | 4 | $q<A<B<C$ | $B$ | $A-q/2$ | $A$ | $N$ |
| | | | $B$ | $q/2$ | $A$ | $100/010/01\bar{1}$ |
| | | | $-B+q/2$ | $-q/2$ | $-A$ | $100/110/111$ |
| | | | $-B+A-q/2$ | $-A+q/2$ | $-A$ | $100/110/00\bar{1}$ |
| 24 | 2 | $A<B<C$ | $B$ | $A/2$ | $A$ | $N$ |
| | | | $-B+A/2$ | $-A/2$ | $-A$ | $100/110/00\bar{1}$ |
| 25 | 2 | $A<B<C$ | $B$ | $A+p-q$ | $p$ | $N$ |
| | | | $-B$ | $-A+q$ | $-p$ | $100/0\bar{1}0/0\bar{1}\bar{1}$ |
| 26 | 2 | $A<B<C$ | $\nu p+q$ | $A$ | $q$ | $N$ |
| | | | $-\nu p$ | $-A$ | $-q$ | $100/0\bar{1}0/101$ |
| 27 | 2 | $A<B<C$ | $B+\mu(p-q)$ | $A$ | $p$ | $N$ |
| | | | $-B-\nu p+\mu q$ | $-A$ | $-p$ | $100/0\bar{1}0/101$ |
| 28 | 2 | $A<B<C$ | $B+p-\mu q$ | $A+p-q$ | $A$ | $N$ |
| | | | $-B+A+\nu q$ | $-A-p+q$ | $-A$ | $100/110/00\bar{1}$ |

$C_j$ is fulfilled and the equalities

$$\xi=\xi_{jh}\,,\quad \eta=\eta_{jh}\,,\quad \zeta=\zeta_{jh} \tag{5}$$

hold, then

(α) the index of the lattice $L$ is equal to $i_j$ which is greater than 1;

(β) $A, B, C, \xi_{j1}, \eta_{j1}, \zeta_{j1}$

. . . . . . . . . . . . . . . . . . . . . .

$A, B, C, \xi_{ji_j}, \eta_{ji_j}, \zeta_{ji_j}$

are all normalized Buerger characteristics of $L$;

(γ) the matrix $\mathsf{M}_{jn}$ $(n=2,\ldots,i_j)$ transforms the cell characterized by

$$A, B, C, \xi_{jn}, \eta_{jn}, \zeta_{jn}$$

into the cell characterized by

$$A, B, C, \xi_{j1}, \eta_{j1}, \zeta_{j1}\,.$$

(*b*) If the numbers $j$, $h$, $p$, $q$ with the properties required in point (*a*) do not exist, then the index of the lattice $L$ is equal to 1 so that (1) is the only normalized Buerger characteristic of $L$.

In simpler words: If we can identify the triplet $\xi, \eta, \zeta$ with a triplet of Table 1 in such a way that the numbers $p$, $q$ satisfy $0<p<q\leq A$ and the corresponding condition is fulfilled then the lattice has more than one Buerger cell. The normalized characteristics of all Buerger cells are listed in the group of rows to which the triplet $\xi, \eta, \zeta$ belongs. If this identification is not possible, the Buerger cell of the lattice is unique.

Three consequences follow immediately from Theorem 3. The first is that the index of any Bravais lattice is not greater than 5. Since all cases from Table 1 really occur, a further statement can be made: if $i$ is an integer fulfilling $1\leq i\leq 5$, then a lattice with the index $i$ may be found.

Secondly, Table 1 shows that in a given Bravais lattice there may be Buerger cells with all acute angles as well as Buerger cells with all obtuse angles. This means that the division of Bravais lattices into two types ('positive' and 'negative') cannot be based on the Buerger cells. The Niggli cell must be applied.

Thirdly, a simple sufficient (but not necessary!) condition may be formulated for a lattice to have the index equal to 1.

*Corollary*. Let (1) be a normalized characteristic of the lattice $L$, let the (sharp) inequalities

$$|\xi|<B\,,\quad |\eta|<A\,,\quad |\zeta|<A$$
$$\xi+\eta+\zeta+A+B>0$$

hold. Then the index of $L$ is equal to 1.

Now let us proceed to the second method.

*Theorem* 4. Let (1) be a normalized Buerger characteristic of the lattice $L$, let the numbers

$$A_k, B_k, C_k, \xi_k, \eta_k, \zeta_k$$

$(k=1,\ldots,25)$ be given by Table 2 where $S=A+B+C$, $\sigma=\xi+\eta+\zeta$. Then the following holds:

(*a*) If

$$A_j+B_j+C_j=A+B+C \tag{6}$$

$(1\leq j\leq 25)$, then

$$A_j, B_j, C_j, \xi_j, \eta_j, \zeta_j \tag{7}$$

is a Buerger characteristic of the lattice $L$.*

(*b*) If

$$A', B', C', \xi', \eta', \zeta' \tag{8}$$

is a normalized Buerger characteristic of the lattice $L$, then an integer $j$ $(1\leq j\leq 25)$ with this property may be

* It need not be normalized.

Table 2. *Potential Buerger characteristics of a lattice*

| $k$ | $A_k$ | $B_k$ | $C_k$ | $\xi_k$ | $\eta_k$ | $\zeta_k$ |
|---|---|---|---|---|---|---|
| 1 | $A$ | $B$ | $C$ | $\xi$ | $\eta$ | $\zeta$ |
| 2 | $A$ | $B$ | $A+C+\eta$ | $\xi+\zeta$ | $2A+\eta$ | $\zeta$ |
| 3 | $A$ | $B$ | $A+C-\eta$ | $-\xi+\zeta$ | $2A-\eta$ | $\zeta$ |
| 4 | $A$ | $B$ | $B+C+\xi$ | $2B+\xi$ | $\eta+\zeta$ | $\zeta$ |
| 5 | $A$ | $B$ | $B+C-\xi$ | $2B-\xi$ | $-\eta+\zeta$ | $\zeta$ |
| 6 | $A$ | $B$ | $S+\sigma$ | $2B+\xi+\zeta$ | $2A+\eta+\zeta$ | $\zeta$ |
| 7 | $A$ | $C$ | $A+B+\zeta$ | $\xi+\eta$ | $2A+\zeta$ | $\eta$ |
| 8 | $A$ | $C$ | $A+B-\zeta$ | $-\xi+\eta$ | $2A-\zeta$ | $\eta$ |
| 9 | $A$ | $C$ | $B+C+\xi$ | $2C+\xi$ | $\eta+\zeta$ | $\eta$ |
| 10 | $A$ | $C$ | $B+C-\xi$ | $-2C+\xi$ | $-\eta+\zeta$ | $\eta$ |
| 11 | $A$ | $C$ | $S+\sigma$ | $2C+\xi+\eta$ | $2A+\eta+\zeta$ | $\eta$ |
| 12 | $A$ | $A+B+\zeta$ | $B+C+\xi$ | $2B+\sigma$ | $\eta+\zeta$ | $2A+\zeta$ |
| 13 | $A$ | $A+B+\zeta$ | $S+\sigma$ | $2A+2B+\sigma+\zeta$ | $2A+\eta+\zeta$ | $2A+\zeta$ |
| 14 | $A$ | $A+B-\zeta$ | $B+C-\xi$ | $-2B+\xi-\eta+\zeta$ | $-\eta+\zeta$ | $2A-\zeta$ |
| 15 | $A$ | $A+C+\eta$ | $S+\sigma$ | $2A+2C+\sigma+\eta$ | $2A+\eta+\zeta$ | $2A+\eta$ |
| 16 | $A$ | $A+C-\eta$ | $B+C-\xi$ | $2C-\xi-\eta+\zeta$ | $-\eta+\zeta$ | $2A-\eta$ |
| 17 | $B$ | $C$ | $A+B+\zeta$ | $\xi+\eta$ | $2B+\zeta$ | $\xi$ |
| 18 | $B$ | $C$ | $A+B-\zeta$ | $-\xi+\eta$ | $-2B+\zeta$ | $\xi$ |
| 19 | $B$ | $C$ | $A+C-\eta$ | $-2C+\eta$ | $-\xi+\zeta$ | $\xi$ |
| 20 | $B$ | $A+B+\zeta$ | $S+\sigma$ | $2A+2B+\sigma+\zeta$ | $2B+\xi+\zeta$ | $2B+\zeta$ |
| 21 | $B$ | $A+B-\zeta$ | $A+C-\eta$ | $2A+\xi-\eta-\zeta$ | $-\xi+\zeta$ | $-2B+\zeta$ |
| 22 | $B$ | $A+C-\eta$ | $B+C-\xi$ | $2C-\xi-\eta+\zeta$ | $2B-\xi$ | $-\xi+\zeta$ |
| 23 | $C$ | $A+B-\zeta$ | $A+C-\eta$ | $2A+\xi-\eta-\zeta$ | $-2C+\eta$ | $-\xi+\eta$ |
| 24 | $C$ | $A+B-\zeta$ | $B+C-\xi$ | $-2B+\xi-\eta+\zeta$ | $-2C+\xi$ | $-\xi+\eta$ |
| 25 | $C$ | $A+C+\eta$ | $S+\sigma$ | $2A+2C+\sigma+\eta$ | $2C+\xi+\eta$ | $2C+\eta$ |

found: If we normalize the sequence (7), we get the sequence (8).

More plainly: If we pick all the $j$'s from Table 2 for which (6) is true and normalize the corresponding sequences (7), we get all normalized Buerger characteristics of the lattice $L$ (some of them, possibly, several times). We have always to go through the whole of Table 2, unlike Table 1 where we stop when the numbers $j$, $h$, $p$, $q$ are found. The data of Table 2 can be stored in a computer and therefore the method is particularly convenient when the lattice is given numerically.

## Niggli cell

The cell based on the reduction of positive definite quadratic forms will be referred to as the Niggli cell. It has an enormous advantage over all other kinds of cells since it is unique. However, it cannot be obtained by means of a simple algorithm and therefore other kinds of cells have been preferred.

The relationship between the Niggli and Buerger cell is simple. The Niggli cell is always a Buerger cell, but the opposite is in general not true. We can only state that one (and only one) of the Buerger cells is a Niggli cell. Thus if the index of a lattice is equal to 1, then its Buerger cell is simultaneously a Niggli cell. The above corollary gives sufficient (but not necessary) conditions for a cell to be a Niggli one.

It is, in fact, a matter of convenience which of the Buerger cells is chosen to be the Niggli cell. The commonly accepted conditions are the following:*

$$\begin{aligned}
&\text{if } \xi = B, \quad \text{then} \quad \zeta \le 2\eta, \\
&\text{if } \eta = A, \quad \text{then} \quad \zeta \le 2\xi, \\
&\text{if } \zeta = A, \quad \text{then} \quad \eta \le 2\xi, \\
&\text{if } \xi = -B, \quad \text{then} \quad \zeta = 0, \\
&\text{if } \eta = -A, \quad \text{then} \quad \zeta = 0, \\
&\text{if } \zeta = -A, \quad \text{then} \quad \eta = 0, \\
&\text{if } \xi + \eta + \zeta + A + B = 0, \\
&\qquad\qquad \text{then } 2(A + \eta) + \zeta \le 0.
\end{aligned}$$

Applying them we can easily indicate the Niggli cell if all Buerger cells are known. This was done in Table 1 where the Niggli cells are denoted by the letter $N$. They correspond always to the values $\xi_{k1}$, $\eta_{k1}$, $\zeta_{k1}$ ($k = 1, \ldots, 28$). The remaining Buerger cells may be converted into the Niggli cell by means of the matrices $\mathsf{M}_{kn}$ ($n = 2, \ldots, i_k$). These matrices can be also used for the mutual transformation of two arbitrary Buerger cells (*via* the Niggli cell).

Santoro & Mighell (1970) published a table of transformation matrices which enable one to find the Niggli cell if a Buerger cell of the lattice is known. However, their procedure does not yield in general the Niggli cell by the first application and reiterations may be necessary.

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* Supposing (1) is a normalized characteristic of the Buerger cell in question.

## Indices of particular lattices

The application of the Niggli forms enables one to ascertain the index of any of the 14 types of Bravais lattice. Table 3 shows the result. The conditions in parentheses (relating to the conventional cell) are necessary and sufficient for the preceding index to occur. However, for monoclinic and triclinic lattices these conditions are not explicitly written, since they are too complicated. Besides the conventional cell is here not unique unless additional conditions are imposed.

Table 3. *Indices of the* 14 *types of Bravais lattice*

| Lattice type | Index |
|---|---|
| Simple cubic | 1 |
| Face-centred cubic | 2 |
| Body-centred cubic | 1 |
| Simple tetragonal | 1 |
| Body-centred tetragonal* | 1, 2 ($2a^2 = 3c^2$) |
| Simple orthorhombic | 1 |
| Base-centred orthorhombic | 1 |
| Face-centred orthorhombic† | 1, 2 ($3a^2 = b^2$) |
| Body-centred orthorhombic† | 1, 2 ($3a^2 - b^2 < c^2 < 3b^2 - a^2$)<br>3 ($3a^2 = b^2 + c^2$ or $3b^2 = a^2 + c^2$) |
| Hexagonal | 1 |
| Trigonal | 1, 2 ($\alpha < 60°$) |
| Simple monoclinic | 1 |
| Base-centred monoclinic | 1, 2, 3 |
| Triclinic | 1, 2, 3, 4, 5 |

* Assuming $a = b$
† Assuming $a < b < c$

On the whole it is apparent that the ambiguity of the Buerger cells – though not exceptional – is not particularly frequent which may, perhaps, account for the fact that it was discovered relatively late and not in full extent. In seven of the 14 types the Buerger cell is always unique; in three types it is either unique or double; in one type (f.c.c.) there are always two different Buerger cells. No more than three types possess the index 3 and the highest values 4 and 5 are reserved for triclinic lattices only.

## Example

Suppose the lattice $L$ has a primitive cell characterized by

$$\begin{aligned}
a &= 2{\cdot}000, & b &= 11{\cdot}66, & c &= 8{\cdot}718, \\
\alpha &= 139°40', & \beta &= 152°45', & \gamma &= 19°24'.
\end{aligned}$$

Then

$$A = 4,\ B = 136,\ C = 76,\ \xi = \overline{155},\ \eta = \overline{31},\ \zeta = 44$$

stands for a characteristic of this lattice the error being nowhere greater than 0·05%. Applying the Algorithms $N$ and $B$ according to Theorem 2 we get successively

| | $A$ | $B$ | $C$ | $\xi$ | $\eta$ | $\zeta$ | $j$ |
|---|---|---|---|---|---|---|---|
| $N2$ | 4 | 136 | 76 | $\overline{155}$ | $\overline{31}$ | 44 | |
| $N3$ | 4 | 76 | 136 | $\overline{155}$ | 44 | $\overline{31}$ | |
| $B2$ | 4 | 76 | 136 | 155 | 44 | 31 | |
| $N2$ | 4 | 76 | 57 | 3 | 13 | 31 | 1 |
| $B3$ | 4 | 57 | 76 | 3 | 31 | 13 | |
| $N2$ | 4 | 57 | 16 | $\overline{49}$ | $\bar{1}$ | 13 | 4 |
| $N3$ | 4 | 16 | 57 | $\overline{49}$ | 13 | $\bar{1}$ | |
| $B2$ | 4 | 16 | 57 | 49 | 13 | 1 | |
| $N3$ | 4 | 16 | 23 | $\overline{15}$ | 11 | 1 | 2 |
| $B3$ | 4 | 16 | 23 | $\overline{15}$ | $\overline{11}$ | $\bar{1}$ | |
| $N2$ | 4 | 16 | 16 | $\overline{16}$ | $\bar{3}$ | $\bar{1}$ | $\bar{1}$ |
| | 4 | 16 | 16 | $\overline{16}$ | $\bar{1}$ | $\bar{3}$ | |

The first column indicates the points of the algorithms which are applied to the sequences in the same row. Since $N2$, $N3$ mean merely change of values and signs, we have actually carried out 4 steps: $B2$, $B3$, $B2$, $B3$. The values 4 and 2 of the $j$ show that the application of the function entier has saved four other steps.

The final sequence

$$4,\ 16,\ 16,\ \overline{16},\ \bar{1},\ \bar{3} \tag{9}$$

is a normalized Buerger characteristic of $L$. If we take notice of the fact that for these values

$$A < B = C\,, \quad \xi = -B\,,$$

we can soon ascertain, running through Table 1, that (5) is fulfilled for $j=20$, $h=3$, $q=2$. The condition $C_{20}$ and the inequalities $0 < p < q \le A$ demanded in Theorem 3 are satisfied. (The value $p$ may be taken arbitrarily, since it does not intervene.) The value $i_{20}=5$ indicates the index of the lattice. All its normalized Buerger characteristics are:

$$\begin{array}{l} 4,\ 16,\ 16,\ 16,\ 3,\ 4\ \ N \\ 4,\ 16,\ 16,\ 16,\ 1,\ 4 \\ 4,\ 16,\ 16,\ \overline{16},\ \bar{1},\ \bar{3} \\ 4,\ 16,\ 16,\ \overline{15},\ \bar{1},\ \bar{4} \\ 4,\ 16,\ 16,\ \overline{13},\ \bar{3},\ \bar{4}\,. \end{array} \tag{10}$$

The first corresponds to the Niggli cell. The shapes of the 5 different Buerger cells are:

| | $a$ | $b$ | $c$ | $\alpha$ | $\beta$ | $\gamma$ | |
|---|---|---|---|---|---|---|---|
| $U_1$: | 2 | 4 | 4 | 60°00′ | 79°12′ | 75°31′ | $N$ |
| $U_2$: | 2 | 4 | 4 | 60°00′ | 86°25′ | 75°31′ | |
| $U_3$: | 2 | 4 | 4 | 120°00′ | 93°35′ | 100°48′ | |
| $U_4$: | 2 | 4 | 4 | 117°57′ | 93°35′ | 104°29′ | |
| $U_5$: | 2 | 4 | 4 | 113°58′ | 100°48′ | 104°29′ | |

If the Niggli cell $U_1$ is associated with the vectors **a**, **b**, **c**, then the other Buerger cells are associated with the following triplets (make inverse matrices to $\mathsf{M}_{20,2}, \ldots, \mathsf{M}_{20,5}$):

$$\begin{array}{llll} U_2: & \mathbf{a}, & \mathbf{b}, & \mathbf{b}-\mathbf{c} \\ U_3: & \mathbf{a}, & -\mathbf{c}, & -\mathbf{b}+\mathbf{c} \\ U_4: & \mathbf{a}, & -\mathbf{a}+\mathbf{b}, & -\mathbf{b}+\mathbf{c} \\ U_5: & \mathbf{a}, & -\mathbf{a}+\mathbf{b}, & -\mathbf{c}\,. \end{array}$$

Now let us try the second method. We start again with the values (9) and apply Table 2. It is not difficult to find that the equality (6) holds only for these values of $j$: 1, 4, 6, 9, 11. The corresponding sequences are:

$$\begin{array}{l} 4,\ 16,\ 16,\ \overline{16},\ \bar{1},\ \bar{3} \\ 4,\ 16,\ 16,\ 16,\ \bar{4},\ \bar{3} \\ 4,\ 16,\ 16,\ 13,\ 4,\ \bar{3} \\ 4,\ 16,\ 16,\ 16,\ \bar{4},\ \bar{1} \\ 4,\ 16,\ 16,\ 15,\ 4,\ \bar{1}\,. \end{array}$$

Normalizing them we get the sequences (10).

According to the Niggli representation

$$\begin{pmatrix} 4 & 16 & 16 \\ 8 & \frac{3}{2} & 2 \end{pmatrix}$$

(or to Table 3) the lattice is triclinic.

## Proofs

The proof of Theorem 3 is fairly long and tedious and only its outline will be given here. Let

$$\mathbf{a},\ \mathbf{b},\ \mathbf{c} \tag{11}$$

be lattice vectors of the lattice $L$; let the equalities (2) hold. Then we say that (11) is a basis (or, alternatively, a Buerger basis) of the lattice $L$, if (1) is a characteristic (Buerger characteristic) of $L$. We say that the vectors (11) are normalized, if (1) is normalized.

Our idea is to compile an auxiliary table which would list (under the given conditions) for any normalized Buerger basis all remaining normalized Buerger bases of the same lattice. It should then be possible, starting from this auxiliary table, to reach Table 1.

Thus, in the first place, we are interested in the relationship between two normalized Buerger bases of a lattice. If (11) and

$$\mathbf{a}',\ \mathbf{b}',\ \mathbf{c}' \tag{12}$$

are two such bases, then

$$\begin{aligned} \mathbf{a}' &= m_{11}\mathbf{a} + m_{12}\mathbf{b} + m_{13}\mathbf{c} \\ \mathbf{b}' &= m_{21}\mathbf{a} + m_{22}\mathbf{b} + m_{23}\mathbf{c} \\ \mathbf{c}' &= m_{31}\mathbf{a} + m_{32}\mathbf{b} + m_{33}\mathbf{c} \end{aligned} \tag{13}$$

with integral coefficients $m_{ik}$, and the determinant equal to $\pm 1$ may be written. But somewhat more can be stated.

*Lemma* 1. Let (11), (12) be normalized Buerger bases of the lattice $L$; let (13) hold. Then the numbers $m_{ik}$ $(i,k=1,2,3)$ assume only the values $1, 0, \bar{1}$.

*Lemma* 2. Let (11) be a normalized Buerger basis of the lattice $L$, $h,k,l$ integers, $\mathbf{r}=h\mathbf{a}+k\mathbf{b}+l\mathbf{c}$. In this case

$$\text{if } l \neq 0\,, \quad \text{then } |\mathbf{r}| \ge |\mathbf{c}|\,,$$
$$\text{if } l = 0\,, \quad k \neq 0\,, \quad \text{then } |\mathbf{r}| \ge |\mathbf{b}|\,.$$

These two lemmas are the main tools for the construction of the auxiliary table. They have been proved by the author (Gruber, 1970).

Hence in the course of this proof we shall assume that (11), (12) are two normalized Buerger bases of a lattice $L$. Notation (2) will be applied. Analogously we denote

$$A'=\mathbf{a}'^2,\quad B'=\mathbf{b}'^2\quad C'=\mathbf{c}'^2$$
$$\xi'=2\mathbf{b}'\,.\,\mathbf{c}',\quad \eta'=2\mathbf{a}'\,.\,\mathbf{c}'\quad ,\ \zeta'=2\mathbf{a}'\,.\,\mathbf{b}'$$

so that

$$A=A',\quad B=B',\quad C=C'. \tag{14}$$

The proof falls into four parts according to the inequalities

$$A=B=C\,,\quad A=B<C\,,\quad A<B=C\,,\quad A<B<C\,. \tag{15}$$

We shall consider the second case

$$A=B<C \tag{16}$$

the others being analogous. According to (3) and (4) either

$$0<\xi\le\eta\le A\,,\quad 0<\zeta\le A \tag{17}$$

or

$$-A\le\eta\le\xi\le 0\,,\quad -A\le\zeta\le 0\,,\quad \xi+\eta+\zeta+2A\ge 0\,. \tag{18}$$

Similar inequalities are valid for the quantities $\xi'$, $\eta'$, $\zeta'$. (A sketch illustrating the set of all points $[\xi,\eta,\zeta]$ fulfilling (17), or alternatively (18) is useful at this point.)

From Lemmas 1 and 2 it follows that any of the vectors $\mathbf{a}'$, $\mathbf{b}'$ must assume one of the following 8 values:

$$\delta\mathbf{a},\quad \delta\mathbf{b},\quad \delta\mathbf{a}+\Delta\mathbf{b}\quad (|\delta|=|\Delta|=1)\,. \tag{19}$$

For the vector $\mathbf{c}'$ we have at most these 18 possibilities

$$\delta\mathbf{c},\quad \delta\mathbf{a}+\Delta\mathbf{c}\,,\quad \delta\mathbf{b}+\Delta\mathbf{c}\,,\quad \delta\mathbf{a}+\Delta\mathbf{b}+\Lambda\mathbf{c}\quad (|\delta|=|\Delta|=|\Lambda|=1)\,.$$

But the cases

$$\mathbf{c}'=\delta\mathbf{a}+\Delta\mathbf{b}+\Lambda\mathbf{c}$$

where either $\delta\neq\Delta$ or $\delta\neq\Lambda$ are in fact excluded. If it were, *e.g.*,

$$\mathbf{c}'=\mathbf{a}+\mathbf{b}-\mathbf{c} \tag{20}$$

we should get [squaring (20) and using (14), (16)]

$$\xi+\eta-\zeta-2A=0$$

which is not in agreement with (17), (18). Thus 12 possibilities

$$\delta\mathbf{c}\,,\quad \delta\mathbf{a}+\Delta\mathbf{c}\,,\quad \delta\mathbf{b}+\Delta\mathbf{c}\,,\quad \delta(\mathbf{a}+\mathbf{b}+\mathbf{c}) \tag{21}$$

remain for $\mathbf{c}'$. The expressions $\delta\mathbf{a}+\Delta\mathbf{b}$ for $\mathbf{a}'$, $\mathbf{b}'$ and

$$\delta\mathbf{a}+\Delta\mathbf{c}\,,\quad \delta\mathbf{b}+\Delta\mathbf{c}\,,\quad \delta(\mathbf{a}+\mathbf{b}+\mathbf{c}) \tag{22}$$

for $\mathbf{c}'$ are rather strong restrictions. If either $\mathbf{a}'$ or $\mathbf{b}'$ is equal to $\delta\mathbf{a}+\Delta\mathbf{b}$, then

$$\zeta=-\delta\Delta A\,. \tag{23}$$

If $\mathbf{c}'$ is equal to the expressions of (22), we get

$$\eta=-\delta\Delta A$$

or

$$\xi=-\delta\Delta A \tag{24}$$

or

$$\xi+\eta+\zeta+2A=0$$

respectively.

Now we have to take all possibilities where $\mathbf{a}'$, $\mathbf{b}'$ assume the values (19) and $\mathbf{c}'$ the values (21) and decide which of them are admissible under the assumption that (11), (12) are normalized Buerger bases of the lattice. Let us perform one case in detail, *e.g.*,

$$\mathbf{a}'=\delta(\mathbf{a}-\mathbf{b})\,,\quad \mathbf{b}'=\Delta\mathbf{a}\,,\quad \mathbf{c}'=\Lambda(\mathbf{b}-\mathbf{c})\,. \tag{25}$$

It must be [see (23), (24)] $\xi=\zeta=A$. Then (17) necessitates $\eta=A$ as well. With these values we get from (25)

$$\xi'=0\,,\quad \eta'=-\delta\Lambda A\,,\quad \zeta'=\delta\Delta A\,.$$

But $\xi'$, $\eta'$, $\zeta'$ must fulfil inequalities similar either to (17) or to (18). This may occur only if $\delta=-\Delta=\Lambda$ and then the determinant of (25) is equal to $\delta$. This means: the relations (25) are valid only if $\xi=\eta=\zeta=A$ and $\delta=-\Delta=\Lambda$, and in this case they transform the normalized Buerger basis (11) into another normalized Buerger basis of the same lattice. In this way one entry of the auxiliary table has been provided. When all possibilities in all four cases (15) are exhausted, the auxiliary table is complete.

Let $K$ denote the number of its entries. The $i$th entry consists of a condition $C_i'$ and two triplets

$$\delta\mathbf{a}_i\,,\quad \delta\mathbf{b}_i\,,\quad \delta\mathbf{c}_i\quad (|\delta|=1)\,. \tag{26}$$

(In the above case $C_i'$ reads $\xi=\eta=\zeta=A=B<C$ and

$$\mathbf{a}_i=\mathbf{a}-\mathbf{b}\,,\quad \mathbf{b}_i=-\mathbf{a}\,,\quad \mathbf{c}_i=\mathbf{b}-\mathbf{c})\,.$$

If the condition $C_i'$ is fulfilled, then, supposing (11) is a normalized Buerger basis of $L$, (26) are also such bases. On the other hand if (11) as well as (12) are normalized Buerger bases of $L$, then such integers $i$, $\delta$ $(1\le i\le K,\ |\delta|=1)$ exist that

$$\mathbf{a}'=\delta\mathbf{a}_i\,,\quad \mathbf{b}'=\delta\mathbf{b}_i\,,\quad \mathbf{c}'=\delta\mathbf{c}_i$$

the condition $C_i'$ being fulfilled.

We do not present here the auxiliary table explicitly since it is too extensive. Applying it we can compile Table 1 for which the propositions of Theorem 3 are true. Thus the proof of this theorem may be considered complete.

The proof of Theorem 4 is based on the auxiliary table as well. First we omit from the auxiliary table all those triplets (26) for which

$$\mathbf{b}_i\,.\,\mathbf{c}_i=\mathbf{b}\,.\,\mathbf{c}\,,\quad \mathbf{a}_i\,.\,\mathbf{c}_i=\mathbf{a}\,.\,\mathbf{c}\,,\quad \mathbf{a}_i\,.\,\mathbf{b}_i=\mathbf{a}\,.\,\mathbf{b}$$

hold supposing (11) is a normalized Buerger basis and the condition $C_i'$ is fulfilled. Then we divide the remaining triplets into classes in this way: two triplets belong to the same class if and only if they either consist of the same vectors (regardless of their order) or if this may be achieved by changing the sign of some vectors of these triplets. Having done this we choose in any class a 'representative triplet' in an arbitrary way and retain it, deleting the remaining triplets from the list. Finally we add the triplet (11). Thus we get a set of 25 triplets. We relabel them from 1 to 25. This relabelling and the choice of the representative triplets may be done in such a way that Table 2 arises if

$$A_k=\mathbf{a}_k^2\,,\quad B_k=\mathbf{b}_k^2\,,\quad C_k=\mathbf{c}_k^2\,,$$
$$\xi_k=2\mathbf{b}_k\,.\,\mathbf{c}_k\,,\quad \eta_k=2\mathbf{a}_k\,.\,\mathbf{c}_k\,,\quad \zeta_k=2\mathbf{a}_k\,.\,\mathbf{b}_k$$

($k=1,\ldots,25$). The construction of this Table shows directly the way to the proof of Theorem 4.

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# The Performances of Neutron Collimators. II. Choice of the Parameters of a Primary Collimator

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The performances of a neutron primary Soller collimator are reviewed, taking into account the finite dimensions of the neutron source. The possibility of choosing suitable values of the parameters to optimize the performances of the collimator, both in intensity and in flux, is shown. A 'figure of merit' for a collimator is discussed. Experimental data are in fair agreement with calculations.

## 1. Introduction

Evaluation of the geometrical parameters of the primary collimator is of utmost importance in the design of a neutron diffractometer or crystal spectrometer, since the intensity transmitted by this collimator strongly affects the overall performance of the experimental set-up.

Szabò (1959, 1960) first studied this problem in detail and Jones (1962) developed a criterion for the optimization of the number of the channels of a Soller collimator when the main geometrical parameters were preset.

In the present work we show that the use of the transmission function of a Soller collimator outlined in a previous paper (Rossitto & Poletti, 1971; this paper will be referred to as NC–I) allows a complete insight into the problem, showing more clearly the dependence of the transmitted intensity on the parameters of the collimator and the influence of the finite dimensions of the neutron source.

We then propose a procedure for choosing the dimensions of the collimator housing and, finally, we define and discuss a 'figure of merit' for the collimator. We also report experiments, whose results fit the calculated values fairly well.

## 2. Transmitted-intensity evaluation

Let $e_h$, $e_v$, $L$ be respectively the width, height and length of a reactor channel (rectangular in section) bounding an isotropic neutron source of density $C$ (neutrons/cm$^2$ . sterad . sec), in which a housing accommodates a Soller collimator of height $h$ and total internal width $s_{tot}$. In the following, $h$ and $s_{tot}$ will be referred to as the collimator-housing parameters. The value of the horizontal angular divergence $\alpha$ has to be set according to the kind of experiment planned and can be obtained simply by choosing a suitable length (and hence number of slits $n$) for the Soller collimator.

First of all, we are interested in determining the collimator geometrical factor $G$, the ratio between the transmitted intensity and the source density $C$. As in

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