To answer the question whether all derived ($hkl0$) origins are in fact F faces, a detailed study of the morphology resulting from the bond strength in the calaverite crystal structure is required. This is not a simple task, even if at present one knows the atomic structure of calaverite, because the microscopic structure of the macroscopically flat faces of an incommensurate crystal is still obscure.

4. Concluding remarks

We still have only a partial understanding of the morphology of calaverite. Nevertheless, the complete indexing of the 92 independent forms of calaverite observed in nature shows the power of the application of the (incommensurate) modulation wave vector as a fourth base vector. The reason for the stability of the satellite faces (see Fig. 3) and the role which the so-called ($hkl0$) origins plays remain unclear, though the extended classical geometrical laws of crystal morphology seem to hold within a reasonable approximation.

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Reduced Cells Based on Extremal Principles

BY B. GRUBER

Faculty of Mathematics and Physics, Charles University, Malostranské nám. 25, 11800 *Prague* 1, *Czechoslovakia*

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Abstract

It is known that the Buerger cell, $a+b+c=$ abs min, is ambiguous. Uniqueness is usually achieved by an additional system of inequalities which leads to the generally accepted Niggli cell. However, this system is rather unusual and does not suggest any geometrical meaning for the Niggli cell. In this paper four types of unique cells originating from the Buerger cell are introduced by means of simple conditions which have an extremal character. Any of these cells may stand for a reduced cell and has an express geometrical property. One of the four types coincides with the Niggli cell, which is thus given a geometrical interpretation. Systems of inequalities are shown that allow recognition of the cell of any type and algorithms are

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presented for achieving it. An algorithm for obtaining all Buerger cells of a lattice is included. The use of the reciprocal lattice enables the definition of four further unique cells which, however, need not be Buerger cells and are not discussed in detail. The mathematics must deal with a number of inequalities which often contain square roots, and sometimes rather intricate technical tricks are required.

Introduction

The problem of a reduced cell may be approached as a problem of a unique representation of a Bravais lattice.

Every cell determines in a unique way that Bravais lattice in which it is embedded. On the other hand any Bravais lattice contains an infinite number of primitive cells differing in shape and size but entirely equivalent for generating the lattice. Thus the problem is to choose one of these cells, the so-called *reduced cell*, which would represent in a certain sense the whole lattice.

The main properties required of a reduced cell are probably the following: it must be (i) unique; (ii) independent of the symmetry of the lattice; (iii) easily recognizable; (iv) accessible by means of an algorithm; and, last but perhaps not least, (v) it ought to have an express geometrical property.* From these standpoints, one may ask how to define a suitable reduced cell.

The clue may perhaps be found when we realize that in a Bravais lattice most of the primitive cells have relatively long edges, large surface, angles nearing zero or 180°, and a long diameter† but only a few show the opposite properties. And since the reduced cell must be unique, it seems sensible to look for it among cells with relatively short edges, small surface, almost right angles, and a short diameter.

Going to the extreme case we may require

$$a+b+c=\text{abs min},\ddagger \tag{1}$$

or

$$\text{surface}=\text{abs min}, \tag{2}$$

or

$$\text{deviation}=\text{abs min}, \tag{3}$$

or

$$\text{diameter}=\text{abs min} \tag{4}$$

where we define

$$\text{deviation}=|\pi/2-\alpha|+|\pi/2-\beta|+|\pi/2-\gamma|.$$

* From this point of view the generally used Niggli cell is - or at least hitherto was - far from being satisfactory. We consider it an important result of this paper that a clear geometrical meaning of the Niggli cell has been found (see the section *Niggli cell*).

† The diameter of a cell is the length of its longest diagonal.

‡ The symbol 'abs' before 'min' indicates that *all* primitive cells of the lattice are taken into account.

Of these four requirements the first is most elaborated. These cells can be characterized by a simple system of inequalities and can be achieved by an algorithm. They are generally called *Buerger cells* and we shall make them the basis and starting point of our investigations. The requirement (2) may be transformed *via* the reciprocal lattice into the first. The questions about conditions (3) and (4) are - as far as we know - open. In a modified form they will give us a clue for further reasoning.

Here a remark concerning notation is relevant. We denote, following general custom,

$$A=\mathbf{a}\,.\,\mathbf{a},\quad B=\mathbf{b}\,.\,\mathbf{b},\quad C=\mathbf{c}\,.\,\mathbf{c},$$
$$D=\mathbf{b}\,.\,\mathbf{c},\quad E=\mathbf{c}\,.\,\mathbf{a},\quad F=\mathbf{a}\,.\,\mathbf{b}$$

and call the sequence

$$A, B, C, D, E, F \tag{5}$$

the *description* of a cell. If the conditions

$$A\le B\le C, \tag{6a}$$
$$\text{if}\quad A=B,\quad\text{then } |D|\le|E|, \tag{6b}$$
$$\text{if}\quad B=C,\quad\text{then } |E|\le|F|, \tag{6c}$$
$$\text{either}\quad D>0,\ E>0,\ F>0 \tag{6d+}$$
$$\text{or}\quad D\le0,\ E\le0,\ F\le0 \tag{6d−}$$

are fulfilled we say that the description (5) is *normalized*. Every cell can be described in a normalized way and this description is unique. Thus, with respect to (6*d*+) and (6*d*−), we can distinguish between *positive* and *non-positive* cells.

A primitive cell described by a normalized sequence (5) is a Buerger cell if and only if the inequalities

$$\begin{gathered}2|D|\le B,\quad 2|E|\le A,\quad 2|F|\le A,\\ A+B+2(D+E+F)\ge0\end{gathered} \tag{7}$$

hold.

Ambiguities of Buerger cells

These cells, with the explicit definition

$$\text{Buerger cell:}\quad a+b+c=\text{abs min},$$

(Buerger, 1957, 1960) meet nicely the requirements (ii) to (v) of the *Introduction* but unfortunately are not unique. This was already known to Eisenstein (though in terms of the quadratic forms) when he published in 1851 a system of additional conditions on how to achieve uniqueness. But a complete analysis was not given until 1973 when a paper by Gruber appeared with a table covering all ambiguities of Buerger cells and giving the number of these cells in every particular case. This list of all ambiguities is essential for our present approach and therefore we reproduce it here in a modified form (Gruber, 1978) as part of Table 1. The exact meaning is given by the following theorem.

Theorem 1

Providing Table 1 is given let (5) be a normalized description of a Buerger cell* of the lattice L. Then the following is true:

(a) If integers k, j ($1 \leq k \leq 24$, $1 \leq j \leq i_k$) may be found such that the conditions $\mathbf{C}_k$, $\mathbf{C}_{kj}$ of Table 1 are fulfilled then the number of different Buerger cells of L is equal to i_k which is a number greater than 1. These Buerger cells are mutually related by the matrices $M_{k1}, \ldots, M_{ki_k}$.†

(b) If such integers k, j cannot be found the Buerger cell of the lattice L is unique.‡

Remark. Let the numbers (5) fulfil the inequalities $0 < A \leq B \leq C$ and some pair $\mathbf{C}_k$, $\mathbf{C}_{kj}$ of the conditions in Table 1. Then (5) may be considered a normalized description of a Buerger cell and theorem 1 may be applied.

Search for uniqueness

Our task is now substantially narrowed: instead of selecting the reduced cell from the infinite number of all primitive cells we have to take it from the set of all Buerger cells, which consists only of at most five cells. The choice must depend in some way or other on the shape of the cell since the edges of all Buerger cells of the same lattice have the same lengths. A simple and natural idea is to characterize the shape by a certain number and then to take that Buerger cell which belongs to the smallest or the greatest value - in the hope that it will be unique.

Thus the final step is to decide on an appropriate characteristic of the shape of the Buerger cells. Which expressions should one try?

First, perhaps, one might try those mentioned in the *Introduction*: S_0 = surface, W_0 = deviation, Φ = diameter.

However, many others may seem suitable, for example

$$S_1 = \sin\alpha + \sin\beta + \sin\gamma,$$
$$S_2 = \sin^2\alpha + \sin^2\beta + \sin^2\gamma,$$
$$S_3 = \sin\alpha \sin\beta \sin\gamma,$$
$$S_4 = |\mathbf{b}\times\mathbf{c}| + |\mathbf{c}\times\mathbf{a}| + |\mathbf{a}\times\mathbf{b}|,$$
$$S_5 = (\mathbf{b}\times\mathbf{c})^2 + (\mathbf{c}\times\mathbf{a})^2 + (\mathbf{a}\times\mathbf{b})^2,$$
$$S_6 = |\mathbf{b}\times\mathbf{c}|\,|\mathbf{c}\times\mathbf{a}|\,|\mathbf{a}\times\mathbf{b}|$$

and similarly

$$W_1 = |\cos\alpha| + |\cos\beta| + |\cos\gamma|,$$
$$W_2 = \cos^2\alpha + \cos^2\beta + \cos^2\gamma,$$
$$W_3 = |\cos\alpha \cos\beta \cos\gamma|,$$
$$W_4 = |\mathbf{b}\,.\,\mathbf{c}| + |\mathbf{c}\,.\,\mathbf{a}| + |\mathbf{a}\,.\,\mathbf{b}|,$$
$$W_5 = (\mathbf{b}\,.\,\mathbf{c})^2 + (\mathbf{c}\,.\,\mathbf{a})^2 + (\mathbf{a}\,.\,\mathbf{b})^2,$$
$$W_6 = |(\mathbf{b}\,.\,\mathbf{c})(\mathbf{c}\,.\,\mathbf{a})(\mathbf{a}\,.\,\mathbf{b})|.$$

Some of them are trivially related:

$$S_4 = S_0/2,$$
$$S_6 = ABCS_3,$$
$$W_2 = 3 - S_2,$$
$$W_5 = BC + CA + AB - S_5,$$
$$W_6 = ABCW_3.$$

Omitting these five as superfluous, we find that ten expressions

$$S_0, S_1, S_2, S_3, S_5, \quad W_0, W_1, W_3, \quad W_4, \Phi \quad (8)$$

remain. For any of these we have ascertained the order of values which correspond to the particular Buerger cells in every one of the 24 ambiguity cases in Table 1. The result is shown in the same table. The order is indicated by the integers 1, 2, 3, ... which start with the greatest value of the expression in question. To equal values the same integer is associated. For example, from Table 1 it follows that*

$$S_0(1,2) > S_0(1,1),$$
$$W_4(10,1) > W_4(10,2) = W_4(10,3).$$

For entry 17 and the expression W_0 three cases are possible:

$$W_0(17,1) > W_0(17,2) > W_0(17,5) > W_0(17,4) > W_0(17,3),$$
$$W_0(17,1) > W_0(17,2) = W_0(17,5) > W_0(17,4) > W_0(17,3),$$
$$W_0(17,1) > W_0(17,5) > W_0(17,2) > W_0(17,4) > W_0(17,3).$$

Which of these occurs may be ascertained from the remarks in Table 1.

The construction of Table 1 constitutes the mathematical crux of this paper. Several hundred inequalities had to be solved on the conditions $\mathbf{C}_k$, $\mathbf{C}_{kj}$. Though many of them were trivial others required elaborate technical tricks and tedious calculations. The details cannot be given here but some suggestions and hints are mentioned in the *Mathematics* section.

* That is, fulfilling (6) and (7).

† To be quite exact, these matrices show possible relations between the Buerger cells but need not be unique, since a certain Buerger cell may occur in the lattice in various positions.

‡ But may possibly be found in several positions.

* The symbol $S_0(k,j)$ means the value of the expression S_0 for the Buerger cell given in the kth entry on the jth line, *etc.*

Table 1. *List of all ambiguities of the Buerger cells, order of values of various expressions and types of cells*

k	i_k	$\mathbf{C}_k$	$\mathbf{C}_{k1},\ldots,\mathbf{C}_{ki_k}$	$M_{k1},\ldots,M_{ki_k}$	S_0	S_1	S_2	S_3	S_5	W_0	W_1	W_3	W_4	Φ	Types
1	2		$0<2D=2E\le 2F=A$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A=2F\le 2E<2D=0$	$\bar{1}00\ 1\bar{1}0\ 001$	1	1	1	1	1	2	2	2	2	2	II, III
2	2	$B<C$	$0<2D=2F<2E=A$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A=2E<2F<2D=0$	$\bar{1}00\ 010\ 10\bar{1}$	1	1	1	1	1	2	2	2	2	2	II, III
3	2	$B<C$	$F<2D<2F<2E=A$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$0<4D<2F<2E=A$	$\bar{1}00\ 0\bar{1}0\ \bar{1}01$	1	1	1	1	1	2	2	2	2	2	II, III
4	2	$A=B$	$0<4D=2E\le 2F=A$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A=2F\le 4D=4E<0$	$010\ 1\bar{1}0\ 00\bar{1}$	1	1	1	1	1	2	2	2	2	2	II, III
5	3	$A=B$	$E<2D<2E\le 2F=A$	$100\ 010\ 001$	3	3	3	3	3	1	1	1	1	1	I, IV
			$0<4D<2E\le 2F=A$	$\bar{1}00\ \bar{1}10\ 00\bar{1}$	2	2	2	2	2	2	2	2	2	2	
			$-A=2F\le 2D+2E<4D<0$	$010\ 1\bar{1}0\ 00\bar{1}$	1	1	1	1	1	3	3	3	3	3	II, III
6	2	$A=B<C$	$0<2F<2D\le 2E=A$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A=2E\le 2D+2F<2F<0$	$\bar{1}00\ 010\ 10\bar{1}$	1	1	1	1	1	2	2	2	2	2	II, III
7	2	$A<B$	$0<2E=2F<A,\ B=2D$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A<2F<2E=B+2D=0$	$100\ 0\bar{1}0\ 01\bar{1}$	1	1	1	1	1	2	2	2	2	2	II, III
8	2	$A<B$	$E<2D<2E\le 2F=A$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$0<4D<2E\le 2F=A$	$\bar{1}00\ \bar{1}10\ 00\bar{1}$	1	1	1	1	1	2	2	2	2	2	II, III
9	2	$A<B$	$0<2E\le 2F=A,\ 2E<2D<B$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A=2F\le 2E<0,\ D<0<B+2D+2E$	$\bar{1}00\ 1\bar{1}0\ 001$	1	1	1	1	1	2	2	2	2	2	II, III
10	3	$A<B$	$A=2E=2F,\ B=2D$	$100\ 010\ 001$	3	3	3	3	3	1	1	1	1	1	I, IV
			$-A-2F=B+2D=E=0$	$100\ \bar{1}10\ 0\bar{1}1$	2	2	2	2	2	3	3	3	2	2	III
			$-A=-B-2D=2E=2F$	$\bar{1}00\ 1\bar{1}0\ 001$	1	1	1	1	1	2	2	2	2	3	II
11	2	$A<B=C$	$0<4E=2F<A,\ B=2D$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A<4E=4F<B+2D=0$	$\bar{1}00\ 001\ 01\bar{1}$	1	1	1	1	1	2	2	2	2	2	II, III
12	2	$A<B=C$	$-K=0<A+2E=A+2F<B+2D$	$100\ 010\ 001$	1	1	1	1	1	1	1	1	1	2	II, IV
			$-K=0<A+2F=B+2D<A+2E$	$\bar{1}00\ 0\bar{1}0\ 111$	2	2	2	2	2	2	2	2	1	1	I, III
13	2	$A<B=C$	$-K=0<A+2F<A+2E=B+2D$	$100\ 010\ 001$	1	1	1	1	1	1	1	1	1	1	II, IV
			$-K=0<B+2D<A+2E=A+2F$	$100\ 001\ \bar{1}\bar{1}\bar{1}$	2	2	2	2	2	2	2	2	1	1	I, III
14	3	$A<B=C$	$A=4E=2F,\ B=2D$	$100\ 010\ 001$	3	3	3	3	3	1	1	1	1	1	I, IV
			$-A=4E=4F,\ B+2D=0$	$\bar{1}00\ 001\ 01\bar{1}$	2	2	2	2	2	3	3	3	2	2	III
			$-A=-2B-4D=4E=2F$	$\bar{1}00\ 1\bar{1}0\ 001$	1	1	1	1	1	2	2	2	2	2	II
15	3	$A<B=C$	$F<2E<2F<A,\ B=2D$	$100\ 010\ 001$	3	3	3	3	3	1	1	1	1	1	I, IV
			$0<4E<2F<A,\ B=2D$	$\bar{1}00\ 0\bar{1}0\ 0\bar{1}1$	2	2	2	2	2	2	2	2	2	2	
			$-B=2D,\ F<E<0<A+2E+2F$	$\bar{1}00\ 001\ 01\bar{1}$	1	1	1	1	1	3	3	3	3	3	II, III
16	3	$A<B=C$	$-K=0<A+2F<A+2E<B+2D$	$100\ 010\ 001$	1	1	1	1	1	1	1	1	1	2	II, IV
			$-K=0<A+2F<B+2D<A+2E$	$\bar{1}00\ 0\bar{1}0\ 111$	2	2	2	2	2	2	2	2	1	1	
			$-K=0<B+2D<A+2F<A+2E$	$100\ 001\ \bar{1}\bar{1}\bar{1}$	3	3	3	3	3	3	3	3	1	1	I, III
17	5	$A<B=C$	$A=2F<4E<2A,\ B=2D$	$100\ 010\ 001$	5	5	5	5	5	111	111	111	1	1	I, IV
			$0<4E<2F=A,\ B=2D$	$\bar{1}00\ 0\bar{1}0\ 0\bar{1}1$	4	4	4	4	4	223	223	223	2	2	
			$-A=2E+2F<4E<B+2D=0$	$\bar{1}00\ 001\ 01\bar{1}$	3	3	3	3	3	545	545	545	3	3	III
			$-A-2F<4E<B+2D+2E=0$	$100\ \bar{1}10\ 0\bar{1}1$	2	2	2	2	2	434	434	434	3	3	
			$-2A<4E<2F=-A,\ B+2D+2E=0$	$\bar{1}00\ 1\bar{1}0\ 001$	1	1	1	1	1	322	322	322	3	4	II
18	2	$A<B<C$	$A=4E=2F,\ B=2D$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A=-2B-4D=4E=2F$	$\bar{1}00\ 1\bar{1}0\ 001$	1	1	1	1	1	2	2	2	2	2	II, III
19	2	$A<B<C$	$F<2E<2F<A,\ B=2D$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$0<4E<2F<A,\ B=2D$	$\bar{1}00\ 0\bar{1}0\ 0\bar{1}1$	1	1	1	1	1	2	2	2	2	2	II, III
20	2	$A<B<C$	$0<2F<2E<A,\ B=2D$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A<2E+2F<2F<B+2D=0$	$100\ 0\bar{1}0\ 01\bar{1}$	1	1	1	1	1	2	2	2	2	2	II, III
21	2	$A<B<C$	$0<2F<2E=A,\ 2F<2D<B$	$100\ 010\ 001$	2	2	2	2	2	1	1	1	1	1	I, IV
			$-A=2E<2F<0,\ D<0<B+2D+2F$	$\bar{1}00\ 010\ 10\bar{1}$	1	1	1	1	1	2	2	2	2	2	II, III
22	2	$A<B<C$	$-K=0<A+2E<B+2D,\ 0<A+2F$	$100\ 010\ 001$	1	1	1	1	1	1	1	1	1	21	II, IV
			$-K=0<B+2D<A+2E,\ 0<A+2F$	$\bar{1}00\ 0\bar{1}0\ 111$	2	2	2	2	2	2	2	2	1	11	I, III
23	3	$A<B<C$	$0<2F<2E=A,\ B=2D$	$100\ 010\ 001$	3	3	3	3	3	1	1	1	1	11	I, IV
			$-A=2E+2F<2E<B+2D=0$	$100\ 0\bar{1}0\ 01\bar{1}$	2	2	2	2	2	3	3	3	2	22	III
			$-A=2E<2F<B+2D+2F=0$	$\bar{1}00\ 010\ 10\bar{1}$	1	1	1	1	1	2	2	2	2	32	II

Table 1 (*cont.*)

k	i_k	$\mathbf{C}_k$	$\mathbf{C}_{k1},\ldots,\mathbf{C}_{ki_k}$	$M_{k1},\ldots,M_{ki_k}$	S_0	S_1	S_2	S_3	S_5	W_0	W_1	W_3	W_4	Φ	Types
24	4	$A<B<C$	$A=2F<4E<2A,\ B=2D$	$100\ 010\ 001$	4	4	4	4	4	111	111	111	1	1	I, IV
			$0<4E<2F=A,\ B=2D$	$\bar{1}00\ 0\bar{1}0\ 0\bar{1}1$	3	3	3	3	3	223	223	223	2	2	
			$-A=2F<4E<B+2D+2E=0$	$100\ \bar{1}10\ 0\bar{1}1$	2	2	2	2	2	434	434	434	3	3	III
			$-2A<4E<2F=-A,\ B+2D+2E=0$	$\bar{1}00\ 1\bar{1}0\ 001$	1	1	1	1	1	322	322	322	3	4	II

Notation: $K=A+B+2(D+E+F)$.

Remarks

(1) Those of the conditions $\mathbf{C}_{kj}$ which determine the non-positive cells begin with a minus sign.

(2) For the expressions W_i ($i=0,1,3$) in entries 17 and 24 the first, or second, or third column is valid if $2E<Q_i$, or $2E=Q_i$, or $2E>Q_i$, respectively, where Q_0 is the (only) root of the function $f(x)=\{(4BC-B^2)[4AC-(A-x)^2]\}^{1/2}-x^2+2Bx-AB-\{[4BC-(B-x)^2](4AC-x^2)\}^{1/2}$ lying between $A/2$ and A, $Q_1=AB^{1/2}/(2B^{1/2}-A^{1/2})$, $Q_3=B-[B(B-A)]^{1/2}$. It is always the case that $A>Q_0>Q_1>Q_3>A/2$. The values (5) relate to the Niggli cell, that is to the first line in entry 17 or 24.

(3) For the expression Φ in entry 22 the first column occurs if $A+E+2F<0$, otherwise the second. In entry 23 the same is true if $A<4F$. The values (5) belong again to the first line.

The four types of reduced cells

A detailed inspection of Table 1 shows various types of behaviour of the expressions (8) with respect to the Buerger cells. But there are some common features which simplify the situation. The main thing in which we are interested is the possibility of defining a unique cell by means of the smallest and the greatest value of the expression in question.

For this purpose W_4 and Φ apparently cannot be used (see *e.g.* entries 13 and 16). The expressions

$$S_0, S_1, S_2, S_3, S_5 \qquad (9)$$

are perfectly suitable, because they always distinguish between two Buerger cells of different shape. This is not always true for the expressions

$$W_0,\ W_1,\ W_3 \qquad (10)$$

(see entries 17 and 24) but, fortunately for us, they still determine in a unique way those cells which correspond to the smallest and the greatest value.

However, the most important thing is that the expressions (9) behave with respect to the Buerger cells 'in the same way'* and thus all determine the same 'minimum cell' and the same 'maximum cell'. This is also done by the expressions (10) although their behaviour with respect to other Buerger cells is more complicated. Let us put it explicitly.

Theorem 2

The expressions

$$\left.\begin{array}{l}\text{surface},\\ \sin\alpha+\sin\beta+\sin\gamma,\\ \sin^2\alpha+\sin^2\beta+\sin^2\gamma,\\ \sin\alpha\sin\beta\sin\gamma,\\ (\mathbf{b}\times\mathbf{c})^2+(\mathbf{c}\times\mathbf{a})^2+(\mathbf{a}\times\mathbf{b})^2\end{array}\right\} \qquad (\mathscr{S})$$

assume their minimum on the set of all Buerger cells of a Bravais lattice for the same cell which therefore is unique. The same is true for their maximum. Similar statements hold for the expressions

$$\left.\begin{array}{l}\text{deviation},\\ |\cos\alpha|+|\cos\beta|+|\cos\gamma|,\\ |\cos\alpha\cos\beta\cos\gamma|.\end{array}\right\} \qquad (\mathscr{D})$$

This opens the way for the following definition.

Definition of four types of unique reduced cells

Type I. Buerger cell with minimum surface:

$$a+b+c=\text{abs min},\ (\mathscr{S})=\text{rel min.}^*$$

Type II. Buerger cell with maximum surface:

$$a+b+c=\text{abs min},\ (\mathscr{S})=\text{rel max.}$$

Type III. Buerger cell with minimum deviation:

$$a+b+c=\text{abs min},\ (\mathscr{D})=\text{rel min.}$$

Type IV. Buerger cell with maximum deviation:

$$a+b+c=\text{abs min},\ (\mathscr{D})=\text{rel max.}$$

These types are indicated in the last column of Table 1. In general they overlap and do *not* constitute a decomposition of the set of all Buerger cells into classes.

Mutual relationships

In any Bravais lattice there are reduced cells of all four types; however, they need not be different. Apparently a Buerger cell belongs to all four types,

$$(\text{I, II, III, IV}),$$

if and only if it is unique. Otherwise it may belong either to one type, or to two types, or to no type (symbol θ). The details are as follows:

(II),	(III),	(I, III),	(I, IV),	(II, III),	(II, IV),	(θ)
5	5	4	20	15	4	6.

The integers in the second row show in how many cases the combination in question occurs in Table 1. It can be seen that the most frequent association is

* That is, $S_p(k,j)<S_p(k,j')$ is equivalent to $S_q(k,j)<S_q(k,j')$ for $0\le p\le 5$, $0\le q\le 5$, $p\ne 4\ne q$, $1\le k\le 24$, $1\le j\le i_k$, $1\le j'\le i_k$.

* The symbol 'rel min' means that only cells fulfilling the condition which precedes are taken into account.

between the types I and IV: they coincide in 20 out of 24 entries of Table 1. We shall find a significant interpretation for this fact in the next section. So much for Buerger cells.

For Bravais lattices eight alternatives concerning the types of the Buerger cells occur:

(I, II, III, IV)	
(I, III), (II, IV)	3
(I, III), (II, IV), (θ)	1
(I, IV), (II, III)	13
(I, IV), (II, III), (θ)	2
(I, IV), (II), (III)	3
(I, IV), (II), (III), (θ)	1
(I, IV), (II), (III), (θ), (θ)	1

For example, the fifth line shows that among the 24 ambiguity cases in Table 1 there are two in which the lattice has one Buerger cell belonging to types I and IV, one Buerger cell belonging to types II and III and one Buerger cell belonging to no type.

Niggli cell

The natural question arises of what is the relationship between our four types and the commonly used Niggli cell (Niggli, 1928). The answer is simple and satisfying:

Theorem 3

The Niggli cell is identical with the cell of type IV, that is, the Niggli cell is the Buerger cell with maximum deviation.

This can be ascertained from Table 1 and the inequalities which define the Niggli cell. Let us put it explicitly.

Theorem 4

A cell of a lattice L is a Niggli cell, if and only if the following extremal conditions are fulfilled:

$$a+b+c=\text{abs min},$$

$$\left.\begin{array}{l}\text{deviation}\\ |\cos\alpha|+|\cos\beta|+|\cos\gamma|\\ |\cos\alpha\cos\beta\cos\gamma|\end{array}\right\}=\text{rel max}.$$

This can also stand for a new definition of the Niggli cell. The author was always puzzled by the discrepancy between the general use and acceptance of the Niggli cell and its somewhat obscure - though logically perfect - definition which does not suggest any sensible geometrical property of this cell. This is now remedied by Theorem 4.

In view of the results of the preceding paragraph the Niggli cell in most cases (but not all) coincides with the Buerger cell with minimum surface. Though a physicist would probably be more inclined to the latter (the surface being more physically significant than the deviation) it can hardly compete with the traditional long-established concept of the Niggli cell.

Table 2. *Determining the type of a Buerger cell*

	Type I	Type IV	Type II	Type III
If $K=0$, $A<B$ then	$G\geq 0$	$G<\dot{0}$	$G<0$	$G\geq 0$
If $K=0$, $A<B=C$ then	$H\geq 0$			$H\geq 0$
If $A=2E$ then	$F<2D$		$F\geq 2D$	
If $A=2F$ then	$E\leq 2D$		$E\geq 2D$, $A<B$	
If $B=2D$ then	$F\leq 2E$		$F\geq 2E$, $B<C$	
If $A+2E=0$ then	$F=0$			
If $A+2F=0$ then	$E=0$			
If $B+2D=0$ then	$F=0$			

Notation: $G=A+2E+F$
$H=A+E+2F$
$K=A+B+2(D+E+F)$.

Recognition

Here we meet the requirement (iii) of the *Introduction*.

Theorem 5

Let (5) be a normalized description of a Buerger cell* of a lattice L. Then the type of this cell - if any - may be ascertained according to Table 2.

This can be verified by means of Table 1, if one also takes the unambiguous cases into account.

Algorithms

Six algorithms are presented here on how to achieve various kinds of cells. The first, algorithm B, starts from an arbitrary primitive cell of the lattice and finds a Buerger cell. Which, however (in ambiguous cases), cannot be specified beforehand. Such algorithms are known (*e.g.* Gruber, 1973, 1978). The present one differs in giving not only the shape but also the position† of the Buerger cell.

Algorithm AB starts from an arbitrary Buerger cell‡ and gives a list of all Buerger cells of the lattice. The types can be recognized according to the values of S_0 and W_0 which are simultaneously computed.

The remaining algorithms TI, TII, TIII, TIV start again from an arbitrary Buerger cell‡ and determine the Buerger cell of the chosen type.§

The position of a cell is related to the reference vectors $\mathbf{a}_0$, $\mathbf{b}_0$, $\mathbf{c}_0$ which need not correspond to a primitive cell. Suitable conventional cells may be chosen. In all algorithms the following notation is used:

$$\mathbf{m}=[m_1, m_2, m_3],$$
$$\mathbf{m}_i=[m_{i1}, m_{i2}, m_{i3}] \quad (1\leq i\leq 5)$$

* That is, fulfilling (6) and (7).
† To be quite exact, one of the possible positions.
‡ And thus can immediately follow algorithm B.
§ Compare TIV with Křivý & Gruber (1976).

and similarly for **n**, **p**. If we are interested only in the parameters of the cell and not in its position, the expressions containing **m**, **n**, **p** can be simply deleted from any algorithm.

All algorithms were tested in all alternatives of the initial values by a computer.

Theorem B

Let

$$\mathbf{a}_0, \mathbf{b}_0, \mathbf{c}_0 \tag{11}$$

be non-coplanar lattice vectors* of a lattice L. Let the vectors

$$\begin{aligned} \mathbf{a} &= m_1\mathbf{a}_0 + m_2\mathbf{b}_0 + m_3\mathbf{c}_0, \\ \mathbf{b} &= n_1\mathbf{a}_0 + n_2\mathbf{b}_0 + n_3\mathbf{c}_0, \\ \mathbf{c} &= p_1\mathbf{a}_0 + p_2\mathbf{b}_0 + p_3\mathbf{c}_0 \end{aligned} \tag{12}$$

determine an *arbitrary primitive cell* of L with the corresponding description (5).† Carry out algorithm B. Then the new values (5) stand for a normalized description of a Buerger cell of the lattice L and (12) (with the new values m_i, n_i, p_i) is one of the possible positions of this cell.

Algorithm B (determining a Buerger cell)

$B0$ Input A, B, C, D, E, F, **m**, **n**, **p**.
$B1$ Carry out sub-algorithm N.
$B2$ If $A<2|F|$, let $j=\text{int}(F/A+0{\cdot}5)$, $B=B+j^2A-2jF$, $D=D-jE$, $F=F-jA$, $\mathbf{n}=\mathbf{n}-j\mathbf{m}$ and go to the point $B1$.
$B3$ If $A<2|E|$, let $j=\text{int}(E/A+0{\cdot}5)$, $C=C+j^2A-2jE$, $D=D-jF$, $E=E-jA$, $\mathbf{p}=\mathbf{p}-j\mathbf{m}$ and go to the point $B1$.
$B4$ If $B<2|D|$, let $j=\text{int}(D/B+0{\cdot}5)$, $C=C+j^2B-2jD$, $D=D-jB$, $E=E-jF$, $\mathbf{p}=\mathbf{p}-j\mathbf{n}$ and go to the point $B1$.
$B5$ Let $K=A+B+2(D+E+F)$, $M=A+B+2F$.
$B6$ If $K<0$, let $j=\text{int}[K/(2M)]$, $C=C+j^2M-2j(D+E)$, $D=D-j(B+F)$, $E=E-j(A+F)$, $\mathbf{p}=\mathbf{p}-j(\mathbf{m}+\mathbf{n})$ and go to the point $B1$.
$B7$ Output: A, B, C, D, E, F, **m**, **n**, **p**.

Theorem AB

Let (11) be non-coplanar lattice vectors* of a lattice L. Let the vectors (12) with the corresponding description (5)† determine a *Buerger cell* of L. Carry out algorithm AB. Then h is the number of all Buerger cells of the lattice L. For $i=1,\dots,h$,

$$A, B, C, D_i, E_i, F_i$$

is the normalized description,

$$\begin{aligned} &m_{i1}\mathbf{a}_0 + m_{i2}\mathbf{b}_0 + m_{i3}\mathbf{c}_0, \\ &n_{i1}\mathbf{a}_0 + n_{i2}\mathbf{b}_0 + n_{i3}\mathbf{c}_0, \\ &p_{i1}\mathbf{a}_0 + p_{i2}\mathbf{b}_0 + p_{i3}\mathbf{c}_0 \end{aligned}$$

one of the possible positions,* S_{0i} the surface, and W_{0i} the deviation of the ith Buerger cell.

Algorithm AB (determining all Buerger cells)

$AB0$ Input A, B, C, D, E, F, **m**, **n**, **p**.
$AB1$ Let $h=0$.
$AB2$ Carry out sub-algorithms N and R.
$AB3$ If $A=2F$, let $D=E-D$, $\mathbf{n}=\mathbf{m}-\mathbf{n}$ and carry out N, R.
$AB4$ If $A=B=2F$, let $E=E-D$, $F=-F$, $\mathbf{m}=\mathbf{m}-\mathbf{n}$ and carry out N, R.
$AB5$ If $A=2E$, let $D=F-D$, $\mathbf{p}=\mathbf{m}-\mathbf{p}$ and carry out N, R.
$AB6$ If $B=2D$, let $E=F-E$, $\mathbf{p}=\mathbf{n}-\mathbf{p}$ and carry out N, R.
$AB7$ If $B=C=2D$, let $D=-D$, $F=F-E$, $\mathbf{n}=\mathbf{n}-\mathbf{p}$ and carry out N, R.
$AB8$ If $A<B$, $A+B+2(D+E+F)=0$, let $D=B+D+F$, $E=A+E+F$, $\mathbf{p}=\mathbf{m}+\mathbf{n}+\mathbf{p}$ and carry out N, R.
$AB9$ If $A<B=C$, $A+B+2(D+E+F)=0$, let $D=B+D+E$, $F=A+E+F$, $\mathbf{n}=\mathbf{m}+\mathbf{n}+\mathbf{p}$ and carry out N, R.
$AB10$ $=AB9$.
$AB11$ If $A+2F=0$, let $D=D+E$, $F=-F$, $\mathbf{n}=\mathbf{m}+\mathbf{n}$ and carry out N, R.
$AB12$ If $A+2E=0$, let $D=D+F$, $E=-E$, $\mathbf{p}=\mathbf{m}+\mathbf{p}$ and carry out N, R.
$AB13$ If $B+2D=0$, let $D=-D$, $E=E+F$, $\mathbf{p}=\mathbf{n}+\mathbf{p}$ and carry out N, R.
$AB14$ If $A<B=2D$, let $E=F-E$, $\mathbf{p}=\mathbf{n}-\mathbf{p}$ and carry out N, R.
$AB15$ If $A=B=2F$, let $D=E-D$, $\mathbf{n}=\mathbf{m}-\mathbf{n}$ and carry out N, R.
$AB16$ Output: h, A, B, C,
D_1, E_1, F_1, S_{01}, W_{01}, $\mathbf{m}_1$, $\mathbf{n}_1$, $\mathbf{p}_1$,
⋮
D_h, E_h, F_h, S_{0h}, W_{0h}, $\mathbf{m}_h$, $\mathbf{n}_h$, $\mathbf{p}_h$.

Theorem T$\mathscr{R}$

Let $\mathscr{R}$ be one of the symbols I, II, III, IV. Let (11) be non-coplanar lattice vectors† of a lattice L. Let the vectors (12) with the corresponding description (5)‡ determine a *Buerger cell* of L. Carry out algorithm $T\mathscr{R}$. Then the new values (5) stand for a normalized description of the cell of the type $\mathscr{R}$ of the lattice L

* They need not belong to a primitive cell of L.
† It need not be normalized.

* It need not coincide with the position given by the matrices $\mathbf{M}_{kj}$ in Table 1.
† They need not belong to a primitive cell of L.
‡ It need not be normalized.

and (12) (with the new values m_i, n_i, p_i) is one of the possible positions* of the cell.

Algorithm TI (*for determining the cell of type* I)

TI0 Input A, B, C, D, E, F, $\mathbf{m}$, $\mathbf{n}$, $\mathbf{p}$.
TI1 Carry out sub-algorithm N.
TI2 If $F<0=B+2D$, let $D=-D$, $E=E+F$, $\mathbf{p}=\mathbf{n}+\mathbf{p}$ and carry out N.
TI3 If $F<0=A+2E$, let $D=D+F$, $E=-E$, $\mathbf{p}=\mathbf{m}+\mathbf{p}$ and carry out N.
TI4 If $E<0=A+2F$, let $D=D+E$, $F=-F$, $\mathbf{n}=\mathbf{m}+\mathbf{n}$ and carry out N.
TI5 If $B=2D$, $2E<F$, let $E=F-E$, $\mathbf{p}=\mathbf{n}-\mathbf{p}$ and carry out N.
TI6 If $A=2E$, $2D<F$, let $D=F-D$, $\mathbf{p}=\mathbf{m}-\mathbf{p}$ and carry out N.
TI7 If $A=2F$, $2D<E$, let $D=E-D$, $\mathbf{n}=\mathbf{m}-\mathbf{n}$ and carry out N.
TI8 If $A<B$, $A+2E+F<0=A+B+2(D+E+F)$, let $D=B+D+F$, $E=A+E+F$, $\mathbf{p}=\mathbf{m}+\mathbf{n}+\mathbf{p}$ and carry out N.
TI9 If $A<B=C$, $A+E+2F<0=A+B+2(D+E+F)$, let $D=B+D+E$, $F=A+E+F$, $\mathbf{n}=\mathbf{m}+\mathbf{n}+\mathbf{p}$ and carry out N.
TI10 Output: A, B, C, D, E, F, $\mathbf{m}$, $\mathbf{n}$, $\mathbf{p}$.

Algorithm TII (*for determining the cell of type* II)

TII0 Input A, B, C, D, E, F, $\mathbf{m}$, $\mathbf{n}$, $\mathbf{p}$.
TII1 Carry out sub-algorithm N.
TII2 If $A=B=2F$, let $E=E-D$, $F=-F$, $\mathbf{m}=\mathbf{m}-\mathbf{n}$ and carry out N.
TII3 If $A=2F<B$, $E<2D$, let $D=E-D$, $\mathbf{n}=\mathbf{m}-\mathbf{n}$ and carry out N.
TII4 If $A=2E$, $F<2D$, let $D=F-D$, $\mathbf{p}=\mathbf{m}-\mathbf{p}$ and carry out N.
TII5 If $B=2D$, $F<2E$, let $E=F-E$, $\mathbf{p}=\mathbf{n}-\mathbf{p}$ and carry out N.
TII6 If $B=C=2D$, let $D=-D$, $F=F-E$, $\mathbf{n}=\mathbf{n}-\mathbf{p}$ and carry out N.
TII7 If $A+B+2(D+E+F)=0<A+2E+F$, let $D=B+D+F$, $E=A+E+F$, $\mathbf{p}=\mathbf{m}+\mathbf{n}+\mathbf{p}$ and carry out N.
TII8 Output: A, B, C, D, E, F, $\mathbf{m}$, $\mathbf{n}$, $\mathbf{p}$.

Algorithm TIII (*for determining the cell of type* III)

TIII$i=T$IIi for $i=0,1,\ldots,6$.
TIII$j=T$I$(j+1)$ for $j=7,8,9$.

Algorithm TIV (*for determining the cell of type* IV)

TIV$i=T$Ii for $i=0,1,\ldots,7$.
TIV$j=T$II$(j-1)$ for $j=8,9$.

* It need not coincide with the position given by the matrices $\mathbf{M}_{kj}$ in Table 1.

Sub-algorithm N (normalization)

$N1$ If $A>B$ or $A=B$, $|D|>|E|$, exchange $A\leftrightarrow B$, $D\leftrightarrow E$, $\mathbf{m}\leftrightarrow\mathbf{n}$.
$N2$ If $B>C$ or $B=C$, $|E|>|F|$, exchange $B\leftrightarrow C$, $E\leftrightarrow F$, $\mathbf{n}\leftrightarrow\mathbf{p}$ and go to the point $N1$.
$N3$ If neither $D>0$, $E>0$, $F>0$ nor $D\le 0$, $E\le 0$, $F\le 0$, let $E=-E$, $F=-F$, $\mathbf{m}=-\mathbf{m}$.
$N4$ If neither $D>0$, $E>0$, $F>0$ nor $D\le 0$, $E\le 0$, $F\le 0$, let $D=-D$, $F=-F$, $\mathbf{n}=-\mathbf{n}$ and go to the point $N3$.
$N5$ Return.

Sub-algorithm R (recording the parameters of the Buerger cells)

$R1$ If $h=0$ or

$$[D, E, F]\neq[D_i, E_i, F_i] \quad \text{for } i=1,\ldots,h,$$

let $h=h+1$,

$$[D_h, E_h, F_h]=[D, E, F],$$
$$\mathbf{m}_h=\mathbf{m},\ \mathbf{n}_h=\mathbf{n},\ \mathbf{p}_h=\mathbf{p},$$
$$S_{0h}=2(BC-D^2)^{1/2}+2(CA-E^2)^{1/2}+2(AB-F^2)^{1/2},$$
$$W_{0h}=1{\cdot}5\pi-\arccos[|D|/(BC)^{1/2}]-\arccos[|E|/(CA)^{1/2}]-\arccos[|F|/(AB)^{1/2}].$$

$R2$ Return.

Reciprocal lattice

The one-to-one correspondence between the primitive cells of a direct lattice L and the primitive cells of its reciprocal lattice L^* makes it possible to define four further types of unique cells which, however, need not be Buerger cells. We shall say that the cell C of the direct lattice L belongs to type I* if the corresponding cell C^* of the reciprocal lattice L^* belongs to type I, and similarly for the other types. An explicit definition reads as follows:

Type I*:
$a^*+b^*+c^*=$ abs min*, surface* = rel min*,†

Type II*:
$a^*+b^*+c^*=$ abs min*, surface* = rel max*,

Type III*:
$a^*+b^*+c^*=$ abs min*, deviation = rel min*,

Type IV*:
$a^*+b^*+c^*=$ abs min*, deviation = rel max*.

This may seem to be a mere formal meaning. But the matter appears in a better light when we realize that the sum $a^*+b^*+c^*$ relating to the cell C^* is

† The symbol 'abs min*' means that all primitive cells of the reciprocal lattice are taken into account, whereas 'rel min*' admits only those cells of L^* which fulfil the preceding condition.

proportional to the surface of the corresponding cell C and *vice versa.* This enables one to write the definitions of types I*, II* in terms of the direct lattice:

Type I*:

surface = abs min, $\quad a+b+c=$ rel min,

Type II*:

surface = abs min, $\quad a+b+c=$ rel max.

Types III* and IV* can be also characterized by the parameters of the direct lattice; however, the expressions are more complicated.

Mathematics

The main feature distinguishing this paper from most other works on Bravais lattices is the use of inequalities instead of equations. Fortunately most of them can be easily solved. Difficulties may arise only with the expressions S_0, S_1 and W_0. The first two lead sometimes to the inequality

$$P_1^{1/2}+Q_1^{1/2}<P_2^{1/2}+Q_2^{1/2}\ (P_i\geq 0,\ Q_i\geq 0,\ i=1,2)$$

which certainly holds if

$$P_1+Q_1<P_2+Q_2,\quad P_1Q_1<P_2Q_2.$$

Surprisingly this sufficient condition, which saves making two further squares, is fulfilled in all our cases.

The expression W_0 can be written

$$\begin{aligned}W_0=1\cdot 5\pi&-\arccos\,[|D|/(BC)^{1/2}]\\&-\arccos\,[|E|/(CA)^{1/2}]\\&-\arccos\,[|F|/(AB)^{1/2}].\end{aligned}$$

The most difficult cases we face here have the form

$$\arccos p_1+\arccos q_1<\arccos p_2+\arccos q_2.$$

The function arccos can be evaded by means of the formula

$$\begin{aligned}&\arccos p+\arccos q\\&=\arccos\,\{pq-[(1-p^2)(1-q^2)]^{1/2}\}\end{aligned}$$

which holds for $0\leq p\leq 1$, $0\leq q\leq 1$.

However, an inequality of the form

$$P+Q^{1/2}\lesseqgtr R^{1/2}\ (P\geq 0,\ Q\geq 0,\ R\geq 0)$$

may still remain. It is equivalent to

$$4P^2Q\lesseqgtr(R-P^2-Q)^2$$

on the assumption that $R\geq P^2+Q$. This can always be verified.

The reader who wants to obtain a better survey of the situation is advised to construct pictures of the sets of points $[D, E, F]$ fulfilling (6), (7) and one of the inequalities

$$0<A=B=C,\quad 0<A=B<C,$$
$$0<A<B=C,\quad 0<A<B<C$$

where A, B, C are considered fixed. These sets are pairs of polyhedra. If (and only if) a point $[D, E, F]$ belongs to one of these polyhedra then (5) stands for a normalized description of a Buerger cell. The conditions $\mathbf{C}_{kj}$ from Table 1 determine simple geometrical figures (points, straight segments, triangles and trapeziums) on the surface of these polyhedra.

Concluding remarks

Any of the eight definitions we have introduced consists of two conditions which are on different levels. The main condition (based on an absolute extreme) selects a small number of cells from the infinite set of all primitive cells, and the additional condition (based on a relative extreme) picks up from these selected cells the final unique reduced cell. Though there cannot be logical objections to such a procedure it seems nevertheless somewhat unsatisfactory. A simple compact geometrically significant one-level condition would probably be preferred – when it is found.

The author thanks his wife for carefully checking his calculations.

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