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Classification of Lattices: a New Step

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Abstract

From the classification of (three-dimensional) lattices into the 14 Bravais types, the finer classifications into the 44 Niggli characters and 24 Delaunay sorts are considered. The last two divisions are mutually incompatible and the Niggli characters show a disturbing 'asymmetry' with respect to the conventional parameters. The aim of the paper is to find a common subdivision of both the Niggli characters and Delaunay sorts that reveals no 'asymmetry'and is crystallographically meaningful. The first attempt based on separating the non-sharp inequalities ($\leq$) into sharp inequalities ($<$) and equalities ($=$) in the systems defining the Niggli characters removed only the 'asymmetry', whereas the incompatibility with the Delaunay sorts remained. The second approach may be called the hyperfaces idea. To any lattice there are attached several points in E_5, its Buerger points. These Buerger points lie in two convex five-dimensional hyperpolyhedra Ω^+, Ω^-. The division of lattices into classes is determined by the distribution of their Buerger points along the vertices, edges, faces, three- and four-dimensional hyperfaces and the interior of Ω^+ and Ω^-. The resulting classes are called genera. There are 127 of them. They form a subdivision of both the Delaunay sorts and the Niggli characters (and, consequently, also of the Bravais types) and their parameter ranges are open. Genera stand for a remarkably strong bond between lattices. The lattices belonging to the same genus agree in a series of important crystallographic properties. Genera are explicitly described by systems of linear inequalities. The five-dimensional geometrical objects obtained in this way are illustrated by their three-dimensional cross sections. From these illustrations, a suitable notation of the genera was derived. Extensive tables enable the determination of the genus of a given lattice.

1. Introduction

If one wants to get an overview over a large (maybe infinite) set of elements, it is helpful to classify the elements into classes, also called types, families, systems, sorts *etc*. Classification means a partition of the set such that each element belongs to exactly one of the classes, *i.e.* the elements must obey the well known equivalence relations. Especially useful is a classification of an infinite set if the number of classes is finite and if the elements belonging to one and the same class have certain properties in common.

(i) The classification of crystal lattices into the 14 Bravais types, often called Bravais lattices, is well known. Less known but also of interest are the finer classifications of lattices into the 44 Niggli characters (*Gitterarten*; Niggli, 1928) and into the 24 Delaunay sorts (*symmetrische Sorten*; Delaunay, 1933*a*,*b*). Both the finer classifications subdivide the Bravais types but are incompatible with each other. This means that lattices of the same character may belong to different Delaunay sorts and lattices of the same Delaunay sort may belong to different Niggli characters. Burzlaff & Zimmermann (1985) have observed this and noted that the correlation between the two classifications is rather low.

(ii) It is not easy to describe the Niggli characters properly (de Wolff, 1988; de Wolff & Gruber, 1991; Gruber, 1992). Following the last author, we characterize any lattice by a unique point in E_5, its Niggli point (see the next section). Then, the division of lattices into the 14 Bravais types means a division of the set Π of all Niggli points into 14 classes. Any of these classes can be – as a subset of E_5 – partitioned into components, *i.e.* maximum connected subsets in the topological sense. It appears that these components correspond to the Niggli characters. Thus, the Niggli characters form *ex definitione* a subdivision of the Bravais types. However, when lattices are described by conventional parameters, the Niggli characters reveal a strange 'asymmetry'. For example, there are two hexagonal Niggli characters, no. 12 when $c/a \geq 1$ and no. 22 when $0 < c/a < 1$. Thus, one range of the parameter c/a is closed and the other open. We consider this situation unsatisfactory and shall make an attempt to remedy it in point (v) of this *Introduction*.

(iii) A different point of view is taken in the definition of the Delaunay sorts. For each lattice, its Voronoi domain can be constructed. It is that region of space whose points are nearer to or at the same distance from a given lattice point P than any other lattice point. All Voronoi domains can be divided according to their shape into five classes, called Voronoi types (Delaunay, 1933*a*,*b*):

(I) cuboctahedron (14 faces, 36 edges, 24 vertices);

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(II) elongated rhomb-dodecahedron (12 faces, 28 edges, 18 vertices);

(III) rhomb-dodecahedron (12 faces, 24 edges, 14 vertices);

(IV) hexagonal prism (8 faces, 18 edges, 12 vertices);

(V) cube (6 faces, 12 edges, 8 vertices).

Within the same Voronoi type, the symmetry of the Voronoi domain varies according to the symmetry of the lattice. Delaunay applied the reduction procedure of Selling (1874), which leads to four lattice vectors with a zero sum and obtuse or right angles. In this way, he obtained a classification of lattices into 24 classes, here called Delaunay sorts. They form a subdivision of the five Voronoi types as well as of the 14 Bravais types.

(iv) Thus, we have two splittings of the Bravais types into finer classes: the 44 Niggli characters and the 24 Delaunay sorts. According to the number of classes, it is not excluded that the Niggli characters form a subdivision of the Delaunay sorts. However, a look at Table 9.3.1 in *International Tables for Crystallography* (1995) (hereafter *IT* A) quickly shows a contradiction to this conjecture: the set of all triclinic lattices is distributed among three Delaunay sorts but there are two Niggli characters only. Later we shall see (Table 5 in this paper) that more often (*i.e.* in 17 cases) lattices of the same Delaunay sort belong to different Niggli characters whereas lattices of the same Niggli character belong to different Delaunay sorts in eight cases. In five cases, the Delaunay sort is identical with a Niggli character. We say that the Niggli characters and Delaunay sorts are incompatible. It is the aim of this paper to find a common subdivision of the Niggli characters and Delaunay sorts that is compatible with both, reveals no 'asymmetry' and is crystallographically meaningful. The 'brute-force' method to subdivide the Niggli characters and Delaunay sorts further with the only aim to remove the incompatibilities is possible, of course, but did not seem to be acceptable to us. (More details about this division are in the section *Building stones*.)

(v) In order to remove the disturbing 'asymmetry' of the Niggli characters and possibly to reduce or remove the number of cases where the lattices of the same Niggli character belong to different Delaunay sorts, we shall try to use the principle of separating the non-sharp inequalities ($\leq$) into sharp inequalities ($<$) and equalities ($=$). The set Π_C of all Niggli points of a particular Niggli character C is a convex k-dimensional ($0 \leq k \leq 5$) hyperpolyhedron and can be described by a system S_C of linear equalities and inequalities between the coordinates of the Niggli points (Gruber, 1992). According to the above principle, any non-sharp inequality ($\leq$) in the system S_C divides this system into two subsystems S_{C1} and S_{C2}, the subsystem S_{C1} having $<$ in the place where $\leq$ was in the system S_C and S_{C2} having $=$. Repeating, if necessary, this procedure for the systems S_{C1}, S_{C2}, we divide eventually S_C into partial subsystems containing only equalities ($=$) and sharp inequalities ($<$) but not non-sharp inequalities ($\leq$). Doing this for all particular Niggli characters, we finally get a division of the set Π of all Niggli points (that is a division of all lattices) into 105 classes with open parameter ranges. According to their definition, they form a subdivision of the Niggli characters. As far as the Delaunay sorts are concerned, we have succeeded only for lattices with Niggli cells with $\alpha, \beta, \gamma \geq 90°$. Among the remaining lattices, there exist classes of the new division with lattices belonging to different Delaunay sorts. Thus, the division is not compatible with the Delaunay sorts and we have to follow another principle.

(vi) Our further approach will be based on the geometrical shape of the set Π of all Niggli points. Before going into details, we introduce the notions that will be needed.

2. Description and representation of a lattice

We say that the cell N determined by a primitive basis

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

of the lattice L is a Buerger cell of L if

$$a + b + c = \text{minimum}$$

on the set of all primitive cells of L. We say that N is a Niggli cell of the lattice L if

(i) N is a Buerger cell of L and

(ii)

$$|90° - \alpha| + |90° - \beta| + |90° - \gamma| = \text{maximum} \tag{2}$$

on the set of all Buerger cells of L (Gruber, 1989). Both cells are primitive. The Niggli cell is unique with regard to its shape (but can occur in different orientations in the lattice) whereas a Buerger cell may be ambiguous (Gruber, 1973). We say that

$$[u, v, x, y, z] \in E_5 \tag{3}$$

is a Niggli point of the lattice L if there exists a Niggli cell N of L and a sequence of vectors (1) in such a way that:

(i) N is determined by the vectors (1);

(ii)

$$u = \mathbf{a}^2/\mathbf{c}^2, \quad v = \mathbf{b}^2/\mathbf{c}^2,$$

$$x = 2\mathbf{b}\cdot\mathbf{c}/\mathbf{c}^2, \quad y = 2\mathbf{a}\cdot\mathbf{c}/\mathbf{c}^2, \quad z = 2\mathbf{a}\cdot\mathbf{b}/\mathbf{c}^2;$$

(iii)

$$u \leq v \leq 1, \tag{4}$$

$$\begin{array}{lll} \text{either} & x > 0, \quad y > 0, \quad z > 0 \\ \text{or} & x \leq 0, \quad y \leq 0, \quad z \leq 0, \end{array} \tag{5}$$

$$\text{if} \quad u = v \quad \text{then} \quad |x| \leq |y|, \tag{6}$$

$$\text{if} \quad v = 1 \quad \text{then} \quad |y| \le |z|. \tag{7}$$

Every lattice has exactly one Niggli point. We shall use it always for the description of the lattice. At present, we use the Niggli point also for the lattice representation but later lattices will be represented in more complicated ways. The Niggli point can be recognized by means of this

Criterion. The point (3) is a Niggli point of a lattice if and only if it fulfils one of the two following systems of inequalities:

(i)

$$u \le v \le 1, \tag{8}$$

$$0 < x \le v, \quad 0 < y \le u, \quad 0 < z \le u,$$

$$\text{if} \quad u = v \quad \text{then} \quad x \le y, \quad \text{if} \quad v = 1 \quad \text{then} \quad y \le z,$$

$$\text{if} \quad x = v \quad \text{then} \quad z \le 2y, \quad \text{if} \quad y = u \quad \text{then} \quad z \le 2x,$$

$$\text{if} \quad z = u \quad \text{then} \quad y \le 2x.$$

(ii)

$$0 < u \le v \le 1, \tag{9}$$

$$-v \le x \le 0, \quad -u \le y \le 0, \quad -u \le z \le 0,$$

$$0 \le u + v + x + y + z,$$

$$\text{if} \quad u = v \quad \text{then} \quad y \le x, \quad \text{if} \quad v = 1 \quad \text{then} \quad z \le y,$$

$$\text{if} \quad x = -v \quad \text{then} \quad z = 0, \quad \text{if} \quad y = -u \quad \text{then} \quad z = 0,$$

$$\text{if} \quad z = -u \quad \text{then} \quad y = 0,$$

$$\text{if} \quad u + v + x + y + z = 0 \quad \text{then} \quad u + y \le v + x$$

(Eisenstein, 1851; Niggli, 1928; *IT* A). The Niggli point of a given lattice can be found by means of an algorithm shown in Appendix *A*.

If the point (3) fulfils the system (8), we speak about a positive Niggli point, if it fulfils the system (9) about a non-positive Niggli point. The set of all Niggli points is denoted Π, the set of all positive Niggli points Π^+ and the set of all non-positive Niggli points Π^-. Thus, $\Pi = \Pi^+ \cup \Pi^-$, $\Pi^+ \cap \Pi^- = \emptyset$.

3. Geometrical relations

The sets Π^+, Π^- are neither open nor closed. It is worth while to introduce Ω^+ as the closure of Π^+ and Ω^- as the closure of Π^- and denote $\Omega = \Omega^+ \cup \Omega^-$. Explicitly, Ω^+ is the set of points (3) fulfilling

$$u \le v \le 1, \tag{10}$$

$$0 \le x \le v, \quad 0 \le y \le u, \quad 0 \le z \le u$$

and Ω^- the set of points (3) fulfilling

$$u \le v \le 1, \tag{11}$$

$$-v \le x \le 0, \quad -u \le y \le 0, \quad -u \le z \le 0,$$

$$0 \le u + v + x + y + z$$

so that $\Omega^+ \cap \Omega^- \neq \emptyset$.

Table 1. *Notation and coordinates of points in E_5*

(*a*) Vertices of the hyperpolyhedra Ω^+ and Ω^-

Ω^+	Ω^-
$\mathbf{0} = [0, 0, 0, 0, 0]$	$\mathbf{0} = [0, 0, 0, 0, 0]$
$\mathbf{1} = [0, 1, 0, 0, 0]$	$\mathbf{1} = [0, 1, 0, 0, 0]$
$\mathbf{2} = [1, 1, 0, 0, 0]$	$\underline{\mathbf{2}} = [1, 1, 0, 0, 0]$
$\mathbf{3} = [0, 1, 1, 0, 0]$	$\underline{\mathbf{3}} = [0, 1, -1, 0, 0]$
$\mathbf{4} = [1, 1, 0, 0, 1]$	$\underline{\mathbf{4}} = [1, 1, 0, 0, -1]$
$\mathbf{5} = [1, 1, 0, 1, 0]$	$\underline{\mathbf{5}} = [1, 1, 0, -1, 0]$
$\mathbf{6} = [1, 1, 0, 1, 1]$	$\underline{\mathbf{6}} = [1, 1, 0. -1, -1]$
$\mathbf{7} = [1, 1, 1, 0, 0]$	$\underline{\mathbf{7}} = [1, 1, -1, 0, 0]$
$\mathbf{8} = [1, 1, 1, 0, 1]$	$\underline{\mathbf{8}} = [1, 1, -1, 0, -1]$
$\mathbf{9} = [1, 1, 1, 1, 0]$	$\underline{\mathbf{9}} = [1, 1, -1, -1, 0]$
$\mathbf{10} = [1, 1, 1, 1, 1]$	

(*b*) Other points of interest

	$\overline{\mathbf{10}} = [1, 1, -2/3, -2/3, -2/3]$
$\mathbf{11} = [1, 1, 1/2, 1, 1]$	$\overline{\mathbf{11}} = [1, 1, -1, -1/2, -1/2]$
$\mathbf{12} = [1, 1, 1, 1/2, 1]$	$\overline{\mathbf{12}} = [1, 1, -1/2, -1/2, -1]$

Both sets, Ω^+ and Ω^-, are closed convex five-dimensional hyperpolyhedra, Ω^+ with 11 and Ω^- with 10 vertices. Their coordinates and notation are given in Table 1. The common part of Ω^+ and Ω^- is the triangle

$$[p, q, 0, 0, 0] \quad (0 \le p \le q \le 1)$$

with the vertices **0**, **1**, **2**.

The boundary of Ω^+ (or Ω^-) consists of vertices and k-dimensional hyperfaces ($1 \le k \le 4$). For our purposes, it is advantageous to take these hyperfaces open with respect to their dimension* so that any two hyperfaces of Ω^+ (or Ω^-) are disjoint. For formal reasons also the vertices and the interior of Ω^+ (or Ω^-) are considered hyperfaces (of the dimension 0 and 5, respectively). In this way, Ω^+ becomes a union of 115 and Ω^- of 119 not overlapping hyperfaces. Seven of them belong to both, Ω^+ and Ω^-, so that the set **H** of all hyperfaces has 227 elements.†

Any hyperface is either a point in E_5 or a k-dimensional hyperpolyhedron ($1 \le k \le 5$) open with respect to its dimension.

4. Notation of hyperfaces

Any hyperface (as a subset of E_5) can be described by a system of linear (in)equalities, for example,

$$0 = u = y = z, \tag{12}$$

$$\begin{aligned} & 0 < x < v < 1 \\ \text{or} \quad & 0 < u < v = 1, \end{aligned} \tag{13}$$

* *I. e.* straight segments without their end points, triangles without their sides and vertices *etc*.

† In detail, Ω^+ (Ω^-) consists of 11 (10) vertices (three of them common), 31 (30) edges (three common), 39 (41) faces (one common), 25 (28) bodies, 8 (9) four-dimensional hyperfaces and 1 (1) five-dimensional interior. This can be ascertained by standard methods of multidimensional analytical geometry. No mathematical difficulties arise. This concerns also some of the further statements that may seem rash at first sight.

$$1+u+x+y+z=0,$$

$$-1<x, \quad -u<y, \quad -u<z.$$

We call these systems fundamental systems. They are consequences of the inequalities (10) or (11) that describe Ω^+ or Ω^-. Some of them will appear explicitly later.

Any of the fundamental systems contains either the equality $u=0$ or one of the four following inequalities:

$$\begin{aligned} 0<u=v=1 &\quad \text{(index 1)},\\ 0<u=v<1 &\quad \text{(index 2)},\\ 0<u<v=1 &\quad \text{(index 3)},\\ 0<u<v<1 &\quad \text{(index 4)}. \end{aligned} \tag{14}$$

They will be distinguished by an index as indicated.

In the first case, *i.e.* $u=0$, we speak about a singular fundamental system* and a singular hyperface. There are altogether 11 of them but they have no importance for us containing no Niggli points.†

Since the five-dimensional space is not accessible to a direct view, we descend to three dimensions. For any u, v $(0<u\le v\le 1)$, we define the points $F_{uv}, \ldots, \Psi_{uv}$ in E_3 according to Table 2.

Now let us keep the values u, v $(0<u\le v\le 1)$ fixed. Then the system of inequalities (10) [or (11)] defines a set $\Omega^+_{uv} \subset E_3$ (or $\Omega^-_{uv} \subset E_3$). These sets are three-dimensional polyhedra, which can be seen in Figs. 1, 2, 3 and 4. Their vertices are described in Table 2. The shape of Ω^+_{uv} when $u=v$ slightly differs from that when $u<v$. The same is true for Ω^-_{uv}. Let us take an arbitrary non-singular fundamental system **F** [*e.g.* the system (13)] and denote the hyperface defined by it as **h**. With the values u, v kept fixed, the system **F** defines a certain subset $\mathbf{h}_{uv}$ of E_3. This set $\mathbf{h}_{uv}$ is a vertex or an open edge or an open face or the interior of the polyhedron Ω^+_{uv} or Ω^-_{uv} and can also be seen in one of Figs. 1, 2, 3 and 4. Because of its shape, $\mathbf{h}_{uv}$ can be uniquely characterized by its vertices. In the case of the system (13), these vertices are

$$K_{uv}, \quad L_{uv}, \quad V_{uv}. \tag{15}$$

Choosing different fixed values u, v, we get different vertices (15), nevertheless, the 'main parts' of their symbols‡ remain the same (in our example K, L, V). Therefore, we shall denote the hyperface **h** by a sequence of these 'main parts' (in alphabetical order) adding as a subscript the index i $(1\le i\le 4)$, which indicates which alternative from (14) occurs in the system **F**. [Thus, the hyperface defined by the system (13) is denoted KLV_3.]

Conversely, having such a symbol, for example

$$JO\Gamma\Delta\Theta\Lambda\Sigma\Psi_2, \tag{16}$$

* Such a system is *e.g.* (12).

† There are the points **0**, **1**, **3**, $\bar{\mathbf{3}}$, the open segments **0 1**, **0 3**, **1 3**, **0** $\bar{\mathbf{3}}$, **1** $\bar{\mathbf{3}}$ and the open triangles **0 1 3**, **0 1** $\bar{\mathbf{3}}$ (see Table 1).

‡ *I.e.* when the subscripts u, v are deleted.

Table 2. *Points in E_3 and their limit positions in E_5*

The indices 1, 2, 3, 4 relate to the four cases in (14). The values u, v fulfil $0<u\le v\le 1$. See Figs. 1, 2, 3 and 4.

Point	Limit positions for the index 1	2	3	4
$F_{uv}=[u/2,u,u]$	**11**	**0, 11**	**1, 11**	**0, 1, 11**
$G_{uv}=[u,u,u]$	**10**	**0, 10**	**1, 10**	**0, 1, 10**
$H_{uv}=[v,u/2,u]$	**12**	**0, 12**	**3, 12**	**0, 3, 12**
$J_{uv}=[v,u,u]$	**10**	**0, 10**	**3, 10**	**0, 3, 10**
$K_{uv}=[-v,0,-u]$	$\bar{\mathbf{8}}$	**0**, $\bar{\mathbf{8}}$	$\bar{\mathbf{3}}$, $\bar{\mathbf{8}}$	**0**, $\bar{\mathbf{3}}$, $\bar{\mathbf{8}}$
$L_{uv}=[-v,-u,0]$	$\bar{\mathbf{9}}$	**0**, $\bar{\mathbf{9}}$	$\bar{\mathbf{3}}$, $\bar{\mathbf{9}}$	**0**, $\bar{\mathbf{3}}$, $\bar{\mathbf{9}}$
$O_{uv}=[0,0,0]$	$\bar{\mathbf{2}}$	**0**, $\bar{\mathbf{2}}$	**1**, $\bar{\mathbf{2}}$	**0, 1**, $\bar{\mathbf{2}}$
$Q_{uv}=[-v,-u/2,-u/2]$	$\overline{\mathbf{11}}$	**0**, $\overline{\mathbf{11}}$	$\bar{\mathbf{3}}$, $\overline{\mathbf{11}}$	**0**, $\bar{\mathbf{3}}$, $\overline{\mathbf{11}}$
$R_{uv}=[-v+u/2,-u/2,-u]$	$\overline{\mathbf{12}}$	**0**, $\overline{\mathbf{12}}$	$\bar{\mathbf{3}}$, $\overline{\mathbf{12}}$	**0**, $\bar{\mathbf{3}}$, $\overline{\mathbf{12}}$
$T_{uv}=[-v+u/3,-2u/3,-2u/3]$	$\overline{\mathbf{10}}$	**0**, $\overline{\mathbf{10}}$	$\bar{\mathbf{3}}$, $\overline{\mathbf{10}}$	**0**, $\bar{\mathbf{3}}$, $\overline{\mathbf{10}}$
$U_{uv}=[0,-u,-u]$	$\bar{\mathbf{6}}$	**0**, $\bar{\mathbf{6}}$	**1**, $\bar{\mathbf{6}}$	**0, 1**, $\bar{\mathbf{6}}$
$V_{uv}=[-v+u,-u,-u]$	$\bar{\mathbf{6}}$	**0**, $\bar{\mathbf{6}}$	$\bar{\mathbf{3}}$, $\bar{\mathbf{6}}$	**0**, $\bar{\mathbf{3}}$, $\bar{\mathbf{6}}$
$X_{uv}=[-v,0,0]$	$\bar{\mathbf{7}}$	**0**, $\bar{\mathbf{7}}$	$\bar{\mathbf{3}}$, $\bar{\mathbf{7}}$	**0**, $\bar{\mathbf{3}}$, $\bar{\mathbf{7}}$
$Y_{uv}=[0,-u,0]$	$\bar{\mathbf{5}}$	**0**, $\bar{\mathbf{5}}$	**1**, $\bar{\mathbf{5}}$	**0, 1**, $\bar{\mathbf{5}}$
$Z_{uv}=[0,0,-u]$	$\bar{\mathbf{4}}$	**0**, $\bar{\mathbf{4}}$	**1**, $\bar{\mathbf{4}}$	**0, 1**, $\bar{\mathbf{4}}$
$\Gamma_{uv}=[0,0,u]$	**4**	**0, 4**	**1, 4**	**0, 1, 4**
$\Delta_{uv}=[0,u,u]$	**6**	**0, 6**	**1, 6**	**0, 1, 6**
$\Theta_{uv}=[v,0,u]$	**8**	**0, 8**	**3, 8**	**0, 3, 8**
$\Lambda_{uv}=[0,u,0]$	**5**	**0, 5**	**1, 5**	**0, 1, 5**
$\Sigma_{uv}=[v,0,0]$	**7**	**0, 7**	**3, 7**	**0, 3, 7**
$\Psi_{uv}=[v,u,0]$	**9**	**0, 9**	**3, 9**	**0, 3, 9**

we describe – following Fig. 2 and Table 2 – by means of inequalities the open hyperpolyhedron in E_3 with the vertices

$$J_{uv}, O_{uv}, \Gamma_{uv}, \Delta_{uv}, \Theta_{uv}, \Lambda_{uv}, \Sigma_{uv}, \Psi_{uv}.$$

In this way, we get the points (3) fulfilling

$$0<x<u, \quad 0<y<u, \quad 0<z<u. \tag{17}$$

Then we add that inequality from (14) that corresponds to the index 2, *i.e.*

$$0<u=v<1. \tag{18}$$

Then (17) together with (18) form a fundamental system that describes the hyperface denoted by the symbol (16).

As can be expected, combining any vertex, edge, face and interior of Ω^+_{uv} and Ω^-_{uv} with any admissible alternative from (14), we get the symbols of all non-singular hyperfaces. It can be easily checked that there are 216 of them, four belonging to Ω^+ as well as to Ω^-. When the 11 singular hyperfaces are added, the total number of 227 hyperfaces is gained. In this way, we can get a fairly clear impression of what the hyperfaces look like and what their mutual relationships are.

It may be asked what are the vertices (in E_5) of a hyperface if its symbol is known. This may be answered by the following limit procedure. From the general condition $0<u\le v\le 1$, three possibilities follow:

(i) $u\to 0$, $v\to 0$,

(ii) $u\to 0$, $v\to 1$,

(iii) $u\to 1$, $v\to 1$.

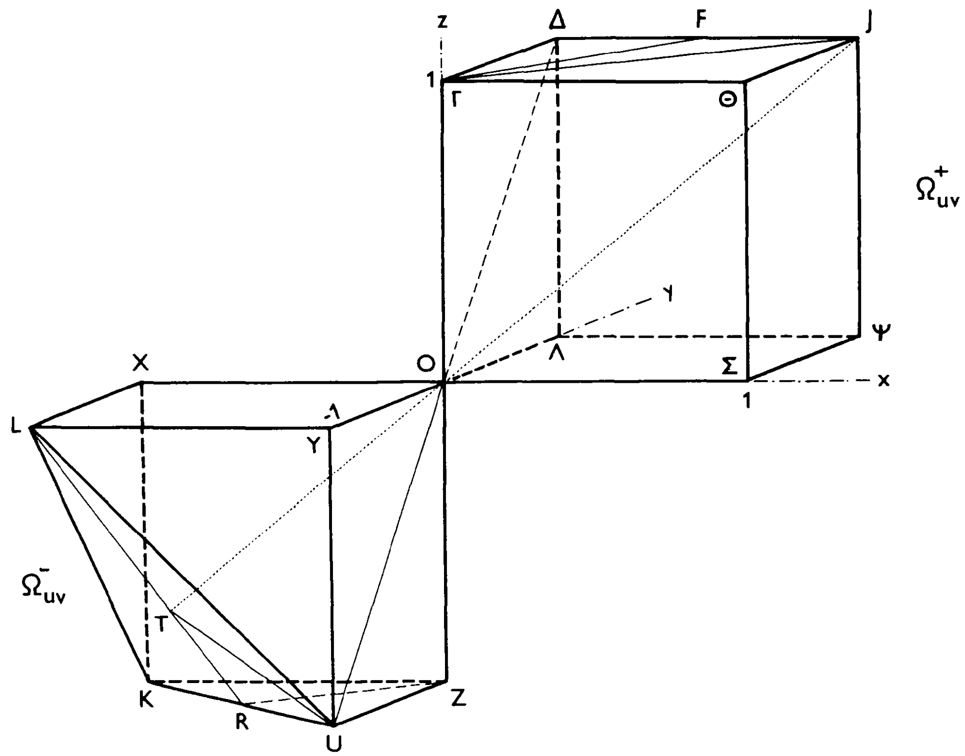

Fig. 1. Three-dimensional illustration of hyperfaces and genera with the index 1, *i.e.* when $u = v = 1$. The polyhedra Ω^+_{uv}, Ω^-_{uv} are three-dimensional cross sections of the five-dimensional hyperpolyhedra Ω^+, Ω^-, supposing the values u, v are considered fixed. The points are described in Table 2, however, their symbols F_{uv}, G_{uv}, ... are simplified in the figure to F, G, ... for graphical reasons. Similarly in Figs. 2, 3 and 4.

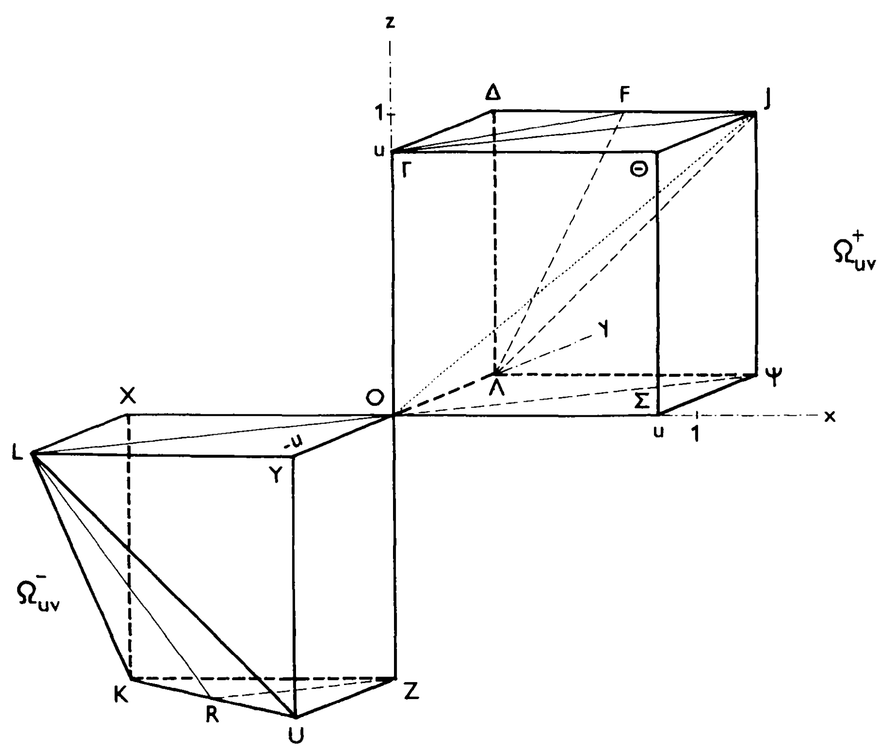

Fig. 2. Three-dimensional illustration of hyperfaces and genera with the index 2, *i.e.* when $0 < u = v < 1$.

However, the limitations imposed on the particular alternatives in (14) allow only the following combinations:
index 1: (iii),
index 2: (i), (iii),
index 3: (ii), (iii),
index 4: (i), (ii), (iii).

Thus, for example, the point $K_{uv} = [-v, 0, -u]$ taken as a point in E_5 (*i.e.* as the point $[u, v, -v, 0, -u]$) can approach under the condition of the index 3 either the point $[0, 1, -1, 0, 0]$ or the point $[1, 1, -1, 0, -1]$, that is either the vertex $\bar{3}$ or the vertex $\bar{8}$ but no others. We express it by $K_3 \rightarrow \bar{3}, \bar{8}$. These limit positions are

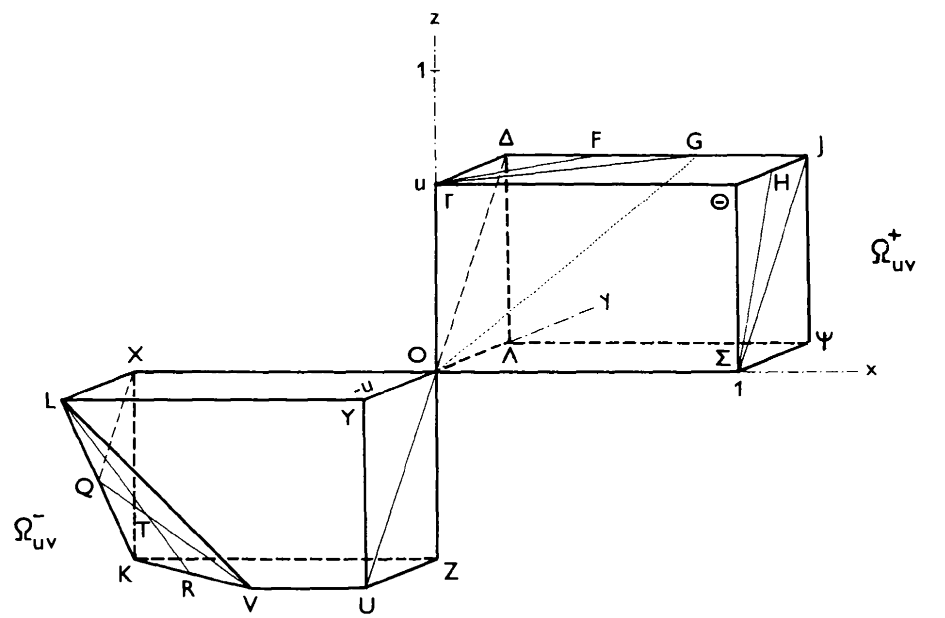

Fig. 3. Three-dimensional illustration of hyperfaces and genera with the index 3, *i.e.* when $0 < u < v = 1$.

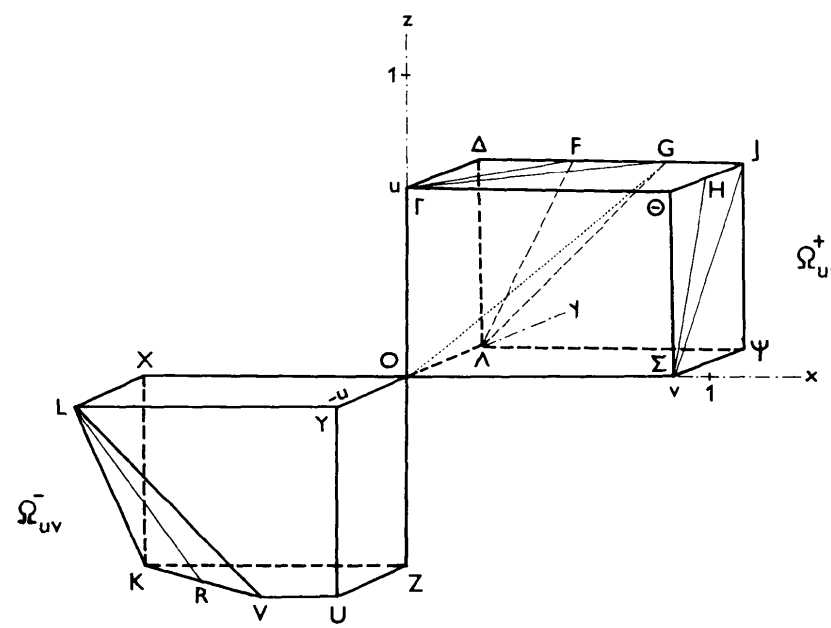

Fig. 4. Three-dimensional illustration of hyperfaces and genera with the index 4, *i.e.* when $0 < u < v < 1$.

recorded in Table 2 for all four indices. According to this table, $L_3 \rightarrow \bar{3}, \bar{9}$, $V_3 \rightarrow \bar{3}, \bar{6}$, from which we deduce that the vertices of the hyperface KLV_3 are $\bar{3}, \bar{6}, \bar{8}, \bar{9}$.

This procedure may be applied to all non-singular hyperfaces. The vertices of the singular hyperfaces must be gained directly from the fundamental systems. For example, the vertices of the hyperface defined by the system (12) are **0**, **1**, **3**.

5. The hyperfaces idea

The system $\mathbf{H}$ of all hyperfaces $\mathbf{h}$ stands for a decomposition of the set Ω into non-overlapping parts. The set Π of all Niggli points is a subset of Ω. Thus, the system of all intersections $\Pi \cap \mathbf{h}$ ($\mathbf{h} \in \mathbf{H}$)* forms a decomposition of Π into non-overlapping parts. This division of the Niggli points induces back a division of lattices. Two lattices belong to the same equivalence class if their Niggli points lie in the same hyperface of Ω^+ or Ω^-. This can be said also like this:

Definition 1. We say that the lattices L_1, L_2 belong to the same class if they agree in the distribution of their Niggli points.†

This formulation shows the relationships with further definitions in a more transparent way. The division of lattices according to this definition consists of 67 classes, which – unlike the Niggli characters – show no 'asymmetrical' phenomena. In this point, we have succeeded. But the classes unfortunately do not form a subdivision of the Bravais types: there are even 27 classes that violate the hierarchy. (For example, the Niggli points [0.8, 0.8, 0.3, 0.6, 0.8], [0.8, 0.8, 0.4, 0.5, 0.8] of the lattices L_1, L_2 both lie in the hyperface $J\Gamma\Delta\Theta_2$, the lattice L_1 being *mC* whereas L_2 is *aP*.)

It is clear that the hyperfaces idea must be refined. The best way to do it is to substitute the Niggli point with another unique point characterizing the lattice. Such a point could be derived, for example, from a cell differing from the Niggli cell in condition (2), which could be substituted by one of the following three conditions:

$$|90^\circ - \alpha| + |90^\circ - \beta| + |90^\circ - \gamma| = \text{minimum}, \quad (19)$$

$$\text{surface of the cell} = \text{maximum}, \quad (20)$$

$$\text{surface of the cell} = \text{minimum}, \quad (21)$$

always on the set of all Buerger cells of the lattice (Gruber, 1989).

However, all these attempts failed leading to the same difficulties. Thus we shall abandon – though with some hesitation – the idea of representing the lattice by a unique point in E_5.

* If the void intersections are omitted.

† Meaning that any hyperface from $\mathbf{H}$ contains the same number (*i.e.* 0 or 1) of Niggli points of L_1 and L_2.

6. Buerger points

The uniqueness of the Niggli point is a consequence of the uniqueness of the Niggli cell and the uniqueness of its description. Thus, we delete the condition (2) [or, possibly, one of the similar conditions (19), (20), (21)] and from the normalizing conditions (4), (5), (6), (7) keep only (4) and modify (5) to be symmetrical.*

Thus, we say that (3) is a Buerger point of the lattice L if there exists a Buerger cell† B of L and a sequence of vectors (1) in such a way that

(i) B is determined by the vectors (1),

(ii)

$$u = \mathbf{a}^2/\mathbf{c}^2, \quad v = \mathbf{b}^2/\mathbf{c}^2, \quad (22)$$

$$x = 2\mathbf{b}\cdot\mathbf{c}/\mathbf{c}^2, \quad y = 2\mathbf{a}\cdot\mathbf{c}/\mathbf{c}^2, \quad z = 2\mathbf{a}\cdot\mathbf{b}/\mathbf{c}^2,$$

(iii)

$$u \le v \le 1, \quad (23)$$

$$\begin{array}{lll} \text{either} & x \ge 0, \quad y \ge 0, \quad z \ge 0 \\ \text{or} & x \le 0, \quad y \le 0, \quad z \le 0. \end{array} \quad (24)$$

A Niggli point is a special case of the Buerger point. A lattice has at least one Buerger point but can have 18 Buerger points.‡ Two lattices have a common Buerger point if and only if they are geometrically similar. Then they have all Buerger points in common. The Buerger points can be easily recognized. They are those points (3) from Ω that have $u > 0$.

To determine one (unspecified) Buerger point of a given lattice L is easy. To find all Buerger points of L is more difficult. However, we need to know them only for constructing the final table of the division of lattices, not when using this table for determining the class to which a particular lattice L belongs. Then only the Niggli point of L must be known. Therefore, we postpone the discussion of how to find all Buerger points of a lattice to Appendix *B*. Now we can modify Definition 1.

Definition 2. We say that the lattices L_1, L_2 belong to the same class if they agree in the distribution of their Buerger points.§

[For example, let $\mathbf{L}$ be the set of lattices with the Niggli points (3) fulfilling $0 < 2x = y < z = u = v < 1$. Then any lattice from $\mathbf{L}$ has two Buerger points in the hyperface $J\Gamma\Delta\Theta_2$ and one Buerger point in the hyperface KUZ_2 but no Buerger points in the remaining hyperfaces. This distribution of Buerger points occurs only for lattices from $\mathbf{L}$. Thus $\mathbf{L}$ forms a class according to Definition 2. It will be denoted later as $F\Gamma_2$.]

* Without (4) and (5), the number of new points would increase enormously.

† *I.e.* a cell fulfilling $a + b + c$ = minimum on the set of all primitive cells of L.

‡ How to prove rash statements like this that occur in many places in the following text is suggested in the section *Proof.*

§ Meaning that any hyperface from $\mathbf{H}$ contains the same number (zero included) of the Buerger points of L_1 and L_2.

What are the properties of this classification of lattices? It consists of 115 classes, is a subdivision of the Bravais types and does not show any 'asymmetry'. In these points, Definition 2 has been successful.

However, we also want the final division to be com patible with the Delaunay sorts and the Niggli characters, that is to be a subdivision of both of them. Here our task has not been accomplished. It turns out that five classes of lattices (according to Definition 2) violate the hierarchy with respect to the Delaunay sorts and another four classes with respect to the Niggli characters. Nevertheless, 106 out of the 115 classes (*i.e.* 92%) fit into both the Delaunay as well as the Niggli partitions. This suggests that the main direction of the reasoning was sensible and definiton 2 only needs to be completed by minor additional conditions.

7. Body diagonals

Let us look more closely at one of the classes that do not fit into the Delaunay sorts. The lattices of this particular class, say **P**, are characterized by Niggli points (3) fulfilling

$$0 < u < v = 1, \quad y = z, \qquad (25)$$
$$0 < x < 1, \quad 0 < y < u.$$

They belong to three Delaunay sorts, namely M_2, M_3 and M_5. This may be ascertained by means of the Delaunay reducing algorithm, his abstract tetrahedron and Fig. 12 of Delaunay (1933*a*,*b*). Asking about the condition for a lattice L of the class **P** to belong to M_2 or M_3 or M_5, we find that it is the (in)equality $x < y$ or $x > y$ or $x = y$, respectively, that relates to the Niggli point (3) of L. But the inequality $x < y$ means the same as

$$|-\mathbf{a}+\mathbf{b}+\mathbf{c}| < |\mathbf{a}-\mathbf{b}+\mathbf{c}|,$$

which is an inequality between the lengths of two body diagonals of the Niggli cell of L. Following this discussion in detail, we find that L belongs to M_2 or to M_3 or to M_5 according to whether the number of the shortest diagonals of the Niggli cell of L is 1, 2 or 3, respectively.

Similar relationships can be found also in the four remaining classes that do not fit into the Delaunay sorts. Therefore, we shall complete definition 2 by the requirement that the lattices of the same class agree in the number of the shortest body diagonals of the Niggli cells.

There is, of course, a question whether this additional condition does not cause a splitting of some classes where it is not necessary, that is which do fit into the Delaunay sorts. A thorough analysis shows that this is not the case.

8. Niggli bases

Now let us draw our attention to the four classes of lattices (according to Definition 2) that do not fit into the Niggli characters. One of these classes – let us denote it **Q** – may be characterized by the following system of inequalities:

$$u = v = 1, \quad 2 + x + y + z = 0, \qquad (26)$$
$$x = y \quad \text{or} \quad y = z, \quad -1 < z < -2/3,$$

which hold for the Niggli points (3) of the lattices from **Q** (and only for them). These lattices belong partly to the Niggli character 6, partly to the Niggli character 7.

Looking for some phenomenon that would enable us to distinguish these two cases, we find after some quest that it may be the bases leading to the Niggli point.

We say that the sequence of vectors (1) is a Niggli basis of the lattice L if

(i) it is a basis of L, and

(ii) the point (3) derived from (1) by means of the relations (22) is a Niggli point of L.

The Niggli basis of a lattice is not unique unlike the Niggli point.

Let us return to our example and ask about the system of all Niggli bases of a lattice L from the class **Q**. It can be shown (see Appendix *C*) that this system always contains the bases

$$\pm(\mathbf{a},\mathbf{b},\mathbf{c}), \quad \pm(\mathbf{b},\mathbf{a},-\mathbf{s}),$$
$$\pm(\mathbf{c},-\mathbf{s},\mathbf{a}), \quad \pm(-\mathbf{s},\mathbf{c},\mathbf{b}),$$

where (1) is an arbitrary Niggli basis of L and $\mathbf{s} = \mathbf{a}+\mathbf{b}+\mathbf{c}$. Besides, this system contains either the bases

$$\pm(\mathbf{b},\mathbf{a},\mathbf{c}), \quad \pm(\mathbf{a},\mathbf{b},-\mathbf{s}), \qquad (27a)$$
$$\pm(\mathbf{c},-\mathbf{s},\mathbf{b}), \quad \pm(-\mathbf{s},\mathbf{c},\mathbf{a})$$

or the bases

$$\pm(\mathbf{a},\mathbf{c},\mathbf{b}), \quad \pm(\mathbf{c},\mathbf{a},-\mathbf{s}), \qquad (27b)$$
$$\pm(\mathbf{b},-\mathbf{s},\mathbf{a}), \quad \pm(-\mathbf{s},\mathbf{b},\mathbf{c})$$

and that is all. In the case (27*a*), the lattice L belongs to the Niggli character 6 [and in (26) $x = y$], in the case (27*b*) to the Niggli character 7 [with $y = z$ in (26)].

A similar situation occurs also in the three remaining classes that do not fit into the Niggli characters. Therefore, we complete Definition 2 by a further requirement, namely that the lattices L_1, L_2 agree in the systems of all Niggli bases. Again, we have to ask whether an unnecessary splitting of classes that do fit into the Niggli characters will occur. Actually, this is not the case.

Like the Buerger points, we shall need the systems of all Niggli bases of a lattice only for constructing the final division of lattices, not when practically seeking the class to which a particular lattice belongs. Therefore, we shall give some hints how to find these systems in Appendix *C*.

9. Genera

Definition 3 (final). We say that the lattices L_1 and L_2 belong to the same class, called a genus, if they agree

(i) in the distribution of their Buerger points,*

(ii) in the number of the shortest body diagonals of their Niggli cells, and

(iii) in the systems of all their Niggli bases.†

This division of lattices is a subdivision of both the Delaunay sorts of symmetry and the Niggli lattice characters (and, consequently, also of the Bravais types). It consists of 127 classes (genera) and is free from 'asymmetrical' phenomena. All parameter ranges are open. We consider it the final division and take it for the solution of our problem.

10. Notation of genera

If **L** is a set of lattices then the set of Niggli points of all lattices from **L** is called the Niggli image of **L**. Thus, we can speak about the Niggli image of a genus. Conversely, this Niggli image defines the genus uniquely. Since the Niggli images of genera are geometrical objects (subsets of E_5), we can describe genera by describing these objects.

The Niggli image of any genus is a part of a hyperface. It is either a point in E_5 or a convex hyperpolyhedron open with respect to its dimension k ($1 \le k \le 5$) or, but only in four cases, a union of at most three such hyperpolyhedra. All these sets can be determined by 'fundamental systems' of inequalities, similarly to the hyperfaces.

Thus, we can describe the Niggli images of genera almost in the same way as the hyperfaces, this time admitting also the symbol $\cup$ for the union of sets. The points in E_5 and E_3 that are needed are described in Tables 1 and 2. The points in E_3 are also illustrated in Figs. 1, 2, 3 and 4.

Bearing in mind the one-to-one correspondence between a genus and its Niggli image, we can use the symbols of the Niggli images of genera also for the genera themselves. These symbols (of all 127 genera) can be found in Tables 3 and 4. They are placed in the column 'Genus'. The preceding column 'Description' serves to determine the fundamental system of the Niggli image of the genus. We must only add to the inequalities from this column one of the inequalities from (14) according to the index that stands as a subscript in the symbol of the genus.

The Niggli images of all genera can be seen in their three-dimensional intersections (when u, v are kept constant) in Figs. 1, 2, 3 and 4. These figures stand for a certain illustration of genera giving at least a limited insight into the relationships between them.

Example. Following Fig. 3 and Table 2, we find that the symbol $GO\Gamma\Delta_3$ denotes the set of points (3) fulfilling

$$u < v = 1,$$
$$0 < x < y < z < u.$$

In a similar way, we find the inequalities

$$u < v = 1,$$
$$0 < y < x < 1,$$
$$y < z < u$$

for the symbol $GJO\Gamma\Theta\Sigma_3$. Thus the Niggli image of the genus

$$GO\Gamma\Delta_3 \cup GJO\Gamma\Theta\Sigma_3 \tag{28}$$

(see Table 3, entry 54) is the set of points (3) fulfilling

$$u < v = 1,$$
$$0 < x < 1, \quad x \ne y,$$
$$0 < y < z < u,$$

which is in agreement with the column 'Description' and with (14).

Table 2 further shows that $GO\Gamma\Delta_3$ is a four-dimensional hyperpolyhedron with the vertices **1**, **2**, **4**, **6**, **10** and $GJO\Gamma\Theta\Sigma_3$ also such a hyperpolyhedron with the vertices **1**, **2**, **3**, **4**, **7**, **8**, **10** both open with respect to the dimension 4. It follows that the Niggli image of the genus (28) may be conceived as an open four-dimensional hyperpolyhedron with the vertices **1**, **2**, **3**, **4**, **6**, **7**, **8**, **10** without the points of the three-dimensional polyhedron with the vertices **1**, **2**, **4**, **10**.

11. Determining the genus of a given lattice

This can be comfortably done by means of Table 3 or Table 4. These tables summarize our main results.

Given a lattice L by means of the parameters of one of its primitive cells, we determine first its Niggli point (3) according to Appendix *A*. We decide whether this point is positive ($x > 0$) or non-positive ($x \le 0$) and according to it apply either Table 3 or Table 4, respectively. Then we compare the requirements of the column 'Determination' with the coordinates of the Niggli point. This must be done going through the entries of the table from the beginning and in the order in which they follow in the table. Then the first agreement gives the genus we are seeking. Its symbol

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* Meaning that any hyperface from **H** contains the same number (zero included) of Buerger points of L_1 and L_2.

† Meaning that if $\mathbf{a}_j$, $\mathbf{b}_j$, $\mathbf{c}_j$ ($j = 1, 2$) are Niggli bases of L_1 and L_2 and if

$$\varphi_i(\mathbf{a}_1, \mathbf{b}_1, \mathbf{c}_1), \quad \psi_i(\mathbf{a}_1, \mathbf{b}_1, \mathbf{c}_1), \quad \chi_i(\mathbf{a}_1, \mathbf{b}_1, \mathbf{c}_1) \quad (i = 1, \ldots, q)$$

are all Niggli bases of L_1 then

$$\varphi_i(\mathbf{a}_2, \mathbf{b}_2, \mathbf{c}_2), \quad \psi_i(\mathbf{a}_2, \mathbf{b}_2, \mathbf{c}_2), \quad \chi_i(\mathbf{a}_2, \mathbf{b}_2, \mathbf{c}_2) \quad (i = 1, \ldots, q)$$

are all Niggli bases of L_2.

Table 3. *Determining the genus: positive Niggli points*

The Niggli point (3) of the lattice fulfils $x > 0$. The first agreement of the values u, v, x, y, z with the conditions in the column 'Determination' determines the genus. Remark: The inequalities in the column 'Description' together with that inequality in (14) whose index is equal to the subscript of the genus symbol check the result. Notation: Ni Niggli lattice character; De Delaunay sort of symmetry; Br Bravais type.

Determination													
u	v	x	y	z	Extra	Description	Genus	Ni	De	Br	Conv. cell		
1	1	1	1	1		$x = y = z = 1$	J_1	1	K_2	cF	$\bar{1}11$	$1\bar{1}1$	$11\bar{1}$
1	1		x	x		$x = y = z$, $0 < x < 1$	JO_1	2	R_2	hR	100	010	001
	u	u	u	u		$x = y = z = u$	J_2	9	R_2	hR	001	$\bar{1}01$	$0\bar{1}1$
1	1		x	1		$x = y, z = 1$, $0 < x < 1$	$J\Gamma_1$	10	M_3	mC	110	$1\bar{1}0$	$00\bar{1}$
1	1		x			$x = y$, $0 < x < z < 1$	$JO\Gamma_1$	10	M_3	mC	110	$1\bar{1}0$	$00\bar{1}$
	u	u	u			$x = y = u$, $0 < z < u$	$J\Psi_2$	10	M_2	mC	110	$1\bar{1}0$	$00\bar{1}$
	u		x	u		$x = y, z = u$, $0 < x < u$	$J\Gamma_2$	10	M_3	mC	110	$1\bar{1}0$	$00\bar{1}$
	u		x	x		$x = y = z$, $0 < x < u$	JO_2	10	M_5	mC	110	$1\bar{1}0$	$00\bar{1}$
	u		x		$x < z$	$x = y$, $0 < x < z < u$	$JO\Gamma_2$	10	M_3	mC	110	$1\bar{1}0$	$00\bar{1}$
	u		x			$x = y$, $0 < z < x < u$	$JO\Psi_2$	10	M_2	mC	110	$1\bar{1}0$	$00\bar{1}$
1	1	1/2	1	1		$2x = y = z = 1$	F_1	18	Q_1	tI	$01\bar{1}$	$1\bar{1}\bar{1}$	100
	1	$u/2$	u	u		$2x = y = z = u$	F_3	18	Q_1	tI	$01\bar{1}$	$1\bar{1}\bar{1}$	100
1	1		1	1		$y = z = 1$, $1/2 < x < 1$	FJ_1	19	O_2	oI	100	$01\bar{1}$	$1\bar{1}\bar{1}$
	1	1	u	u		$x = 1$, $y = z = u$	J_3	19	O_3	oI	100	$01\bar{1}$	$1\bar{1}\bar{1}$
	1	u	u	u		$x = y = z = u$	G_3	19	O_4	oI	100	$01\bar{1}$	$1\bar{1}\bar{1}$
	1		u	u	$x < u$	$y = z = u$, $u/2 < x < u$	FG_3	19	O_2	oI	100	$01\bar{1}$	$1\bar{1}\bar{1}$
	1		u	u		$y = z = u$, $u < x < 1$	GJ_3	19	O_3	oI	100	$01\bar{1}$	$1\bar{1}\bar{1}$
1	1			y		$y = z$, $0 < x < y < 1$	$JO\Delta_1$	20	M_2	mC	011	$01\bar{1}$	$\bar{1}00$
	1	1		y		$x = 1, y = z$, $0 < y < u$	$J\Sigma_3$	20	M_3	mC	011	$01\bar{1}$	$\bar{1}00$
	1		x	x		$x = y = z$, $0 < x < u$	GO_3	20	M_5	mC	011	$01\bar{1}$	$\bar{1}00$
	1			y	$x < y$	$y = z$, $0 < x < y < u$	$GO\Delta_3$	20	M_2	mC	011	$01\bar{1}$	$\bar{1}00$
	1			y		$y = z < u$, $0 < y < x < 1$	$GJO\Sigma_3$	20	M_3	mC	011	$01\bar{1}$	$\bar{1}00$
	u	$u/2$	u	u		$2x = y = z = u$	F_2	26	O_1	oF	100	$1\bar{2}0$	$10\bar{2}$
		$u/2$	u	u		$2x = y = z = u$	F_4	26	O_1	oF	100	$1\bar{2}0$	$10\bar{2}$
	u		u	u		$y = z = u$, $u/2 < x < u$	FJ_2	27	M_2	mC	$1\bar{2}0$	$\bar{1}00$	$01\bar{1}$
		v	u	u		$x = v$, $y = z = u$	J_4	27	M_3	mC	$1\bar{2}0$	$\bar{1}00$	$01\bar{1}$
		u	u	u		$x = y = z = u$	G_4	27	M_5	mC	$1\bar{2}0$	$\bar{1}00$	$01\bar{1}$
			u	u	$x < u$	$y = z = u$, $u/2 < x < u$	FG_4	27	M_2	mC	$1\bar{2}0$	$\bar{1}00$	$01\bar{1}$
			u	u		$y = z = u$, $u < x < v$	GJ_4	27	M_3	mC	$1\bar{2}0$	$\bar{1}00$	$01\bar{1}$
	u		u	$2x$		$2x = z, y = u$, $0 < z < u$	$F\Lambda_2$	28	M_1	mC	100	$10\bar{2}$	$0\bar{1}0$
			u	$2x$		$2x = z, y = u$, $0 < z < u$	$F\Lambda_4$	28	M_1	mC	100	$10\bar{2}$	$0\bar{1}0$
1	1		$2x$	1		$2x = y, z = 1$, $0 < y < 1$	$F\Gamma_1$	29	M_1	mC	100	$1\bar{2}0$	$00\bar{1}$
	u		$2x$	u		$2x = y, z = u$, $0 < y < u$	$F\Gamma_2$	29	M_1	mC	100	$1\bar{2}0$	$00\bar{1}$
	1		$2x$	u		$2x = y, z = u$, $0 < y < u$	$F\Gamma_3$	29	M_1	mC	100	$1\bar{2}0$	$00\bar{1}$
			$2x$	u		$2x = y, z = u$, $0 < y < u$	$F\Gamma_4$	29	M_1	mC	100	$1\bar{2}0$	$00\bar{1}$

Table 3 (*cont.*)

Determination u	v	x	y	z	Extra	Description	Genus	Ni	De	Br	Conv. cell		
	1	1	$u/2$	u		$x = 1$, $2y = z = u$	H_3	30	M_1	mC	010	$01\bar{2}$	$\bar{1}00$
	1	1		$2y$		$x = 1, 2y = z$, $0 < z < u$	$H\Sigma_3$	30	M_1	mC	010	$01\bar{2}$	$\bar{1}00$
		v	$u/2$	u		$x = v$, $2y = z = u$	H_4	30	M_1	mC	010	$01\bar{2}$	$\bar{1}00$
		v		$2y$		$x = v, 2y = z$, $0 < z < u$	$H\Sigma_4$	30	M_1	mC	010	$01\bar{2}$	$\bar{1}00$
1	1			1		$z = 1$, $y/2 < x < y < 1$	$FJ\Gamma_1$	31	T_1	aP	100	010	001
1	1					$0 < x < y$, $y < z < 1$	$JO\Gamma\Delta_1$	31	T_1	aP	100	010	001
	u			u		$z = u$, $y/2 < x < y < u$	$FJ\Gamma_2$	31	T_1	aP	100	010	001
	u		u	x		$x = z, y = u$, $0 < x < u$	$J\Lambda_2$	31	T_2	aP	100	010	001
	u		u		$x < z$	$y = u$, $z/2 < x < z < u$	$FJ\Lambda_2$	31	T_1	aP	100	010	001
	u		u			$y = u$, $0 < z < x < u$	$J\Lambda\Psi_2$	31	T_1	aP	100	010	001
	u			x		$x = z$, $0 < x < y < u$	$JO\Lambda_2$	31	T_2	aP	100	010	001
	u					$x \neq z$, $0 < x < y < u$, $0 < z < u$	*	31	T_1	aP	100	010	001
	1	1		u		$x = 1, z = u$, $u/2 < y < u$	HJ_3	31	T_1	aP	100	010	001
	1	1				$x = 1$, $z/2 < y < z < u$	$HJ\Sigma_3$	31	T_1	aP	100	010	001
	1		x	u		$x = y, z = u$, $0 < x < u$	$G\Gamma_3$	31	T_2	aP	100	010	001
	1			u	$x < y$	$z = u$, $y/2 < x < y < u$	$FG\Gamma_3$	31	T_1	aP	100	010	001
	1			u		$y < z = u$, $0 < y < x < 1$	$GJ\Gamma\Theta_3$	31	T_1	aP	100	010	001
	1		x			$x = y$, $0 < x < z < u$	$GO\Gamma_3$	31	T_2	aP	100	010	001
	1					$x \neq y$, $0 < x < 1$, $0 < y < z < u$	†	31	T_1	aP	100	010	001
		v	u			$x = v, y = u$, $0 < z < u$	$J\Psi_4$	31	T_1	aP	100	010	001
		v		u		$x = v, z = u$, $u/2 < y < u$	HJ_4	31	T_1	aP	100	010	001
		v		y		$x = v, y = z$, $0 < y < u$	$J\Sigma_4$	31	T_2	aP	100	010	001
		v			$y < z$	$x = v$, $z/2 < y < z < u$	$HJ\Sigma_4$	31	T_1	aP	100	010	001
		v				$x = v$, $0 < z < y < u$	$J\Sigma\Psi_4$	31	T_1	aP	100	010	001
			u	x		$x = z, y = u$, $0 < x < u$	$G\Lambda_4$	31	T_2	aP	100	010	001
			u		$x < z$	$y = u$, $z/2 < x < z < u$	$FG\Lambda_4$	31	T_1	aP	100	010	001
			u			$z < y = u$, $0 < z < x < v$	$GJ\Lambda\Psi_4$	31	T_1	aP	100	010	001
			x	u		$x = y, z = u$, $0 < x < u$	$G\Gamma_4$	31	T_2	aP	100	010	001
				u	$x < y$	$z = u$, $y/2 < x < y < u$	$FG\Gamma_4$	31	T_1	aP	100	010	001
				u		$y < z = u$, $0 < y < x < v$	$GJ\Gamma\Theta_4$	31	T_1	aP	100	010	001
			x	x		$x = y = z$, $0 < x < u$	GO_4	31	T_3	aP	100	010	001

Table 3 (*cont.*)

Determination													
u	v	x	y	z	Extra	Description	Genus	Ni	De	Br	Conv. cell		
			x		$x < z$	goto &							
				x	$x < y$	goto &							
				y	$y < x$	goto &							
						& $x = y$, $0 < x < z < u$ or $x = z$, $0 < x < y < u$ or $y = z < u$, $0 < y < x < v$	‡	31	T_2	aP	100	010	001
						$x < y < u$, $0 < x < z < u$ or $y < x < v$, $0 < y < z < u$ or $z < x < v$, $0 < z < y < u$	§	31	T_1	aP	100	010	001

* $JO\Lambda\Psi_2 \cup JO\Gamma\Delta\Lambda_2$. † $GO\Gamma\Delta_3 \cup GJO\Gamma\Theta\Sigma_3$. ‡ $GO\Gamma_4 \cup GO\Lambda_4 \cup GJO\Sigma_4$. § $GO\Gamma\Delta\Lambda_4 \cup GJO\Gamma\Theta\Sigma_4 \cup GJO\Lambda\Sigma\Psi_4$.

is in the column 'Genus'. The column 'Description' and the proper alternative from (14) check our result. Further columns in Tables 3 and 4 determine the Niggli character, the Delaunay sort of symmetry and the Bravais type of the lattice L. In the last column, the conventional cell is given. The matrices relate to a Niggli basis but, of course, are not unique.

Example. Suppose that the lattice L has the Niggli point

$$[0.6, 0.6, -0.24, -0.42, -0.54]. \qquad (29)$$

Going through Table 4, we stop at the 17th entry. It shows that the lattice L belongs to the genus LRU_2. The inequalities from the column 'Description'

$$2u + x + y + z = 0,$$

$$-u < y < x, \quad -u < z$$

together with the inequality indicated by the index 2, *i.e.*

$$0 < u = v < 1,$$

form the fundamental system of the genus LRU_2. This system is fulfilled by the Niggli point (29), which verifies the finding. Table 4 further shows that the lattice L is monoclinic face centered and belongs to the Delaunay sort M_2 and to the Niggli character 17. The vectors $\mathbf{a} - \mathbf{b}$, $\mathbf{a} + \mathbf{b}$, $-\mathbf{a} - \mathbf{c}$ determine the conventional cell.

12. Classification of lattices

Detailed mutual relationships between the four divisions can be obtained from Table 5. All genera belonging to a given Bravais type, Delaunay sort or Niggli character are immediately seen. In particular, the explicit relations between the Delaunay sorts and the Niggli characters, which had not been previously established, are ascertained. Conspicuous is the great number of genera forming the mC and aP Bravais types (43 in both cases).

13. Building stones

The way in which the genera were defined and their fairly great number enable us to use them as building stones for constructing various other divisions of lattices.

For example, the 'minimum common subdivision' of the Delaunay sorts and the Niggli characters (*i.e.* having the smallest number of classes) is a superdivision of genera. From Table 5, it follows that this division has 57 classes. Among them 28 coincide with a genus and have open parameter ranges. The remaining 29 classes consist mostly of 2 but also of 3, 4, 6, 8 and 20 genera, however, their parameter ranges are not open. All classes may be described by the symbols of their genera.

In a similar way, we can ascertain that the (otherwise unimportant) division of lattices according to Definition 2, which has been already mentioned, has 115 classes. Of these, 106 coincide with a genus, 6 consist of two and 3 of three genera. In particular, the class described previously by the inequalities (25) is a union of the genera $GO\Delta_3$, $GJO\Sigma_3$, GO_3 and the class described by (26) a union of the genera RT_1, TU_1.

14. Extension

From a sensible division of an arbitrary set, we usually expect that the elements belonging to the same equivalence class are in some way related, that they have some properties in common. These elements agree, of course, automatically in those properties according to which the division was made. If they agree ('by chance') also in

Table 4. *Determining the genus: non-positive Niggli points*

The Niggli point (3) of the lattice fulfils $x \le 0$. Further, $s = u + v + x + y + z$ and $w = v + x - y$ is set. Then the first agreement of the values u, v, x, y, z, s, w with the conditions in the column 'Determination' determines the genus. Remark: as in caption to Table 3.

Determination												Conv. cell		
u	v	x	y	z	s	w	Description	Genus	Ni	De	Br			
1	1	0	0	0			$x = y = z = 0$	O_1	3	K_3	cP	100	010	001
1	1		x	x	0		$x = y = z$, $x = -2/3$	T_1	5	K_1	cI	011	101	110
1	1		x	x			$x = y = z$, $-2/3 < x < 0$	OT_1	4	R_1	hR	100	010	001
1	1		x		0		$x = y, s = 0$, $-1 < z < -2/3$	RT_1	6	Q_1	tI	101	011	110
1	1			y	0		$y = z, s = 0$, $-2/3 < x < 0$	TU_1	7	Q_1	tI	110	101	011
1	1				0		$s = 0$, $-1 < z < y < x$	RTU_1	8	O_2	oI	110	101	011
	u	0	0	0			$x = y = z = 0$	O_2	11	Q_3	tP	100	010	001
1	1	0	0	-1			$x = y = 0$, $z = -1$	Z_1	12	H	hP	100	010	001
	u	0	0	$-u$			$x = y = 0$, $z = -u$	Z_2	12	H	hP	100	010	001
1	1	0	0				$x = y = 0$, $-1 < z < 0$	OZ_1	13	O_5	oC	110	$1\bar{1}0$	001
	u	0	0				$x = y = 0$, $-u < z < 0$	OZ_2	13	O_5	oC	110	$1\bar{1}0$	001
	u	$-u$	$-u$	0			$x = y = -u$, $z = 0$	L_2	15	Q_2	tI	100	010	112
	u		x		0		$x = y, s = 0$, $-u < z < 0$	LR_2	16	O_1	oF	110	$1\bar{1}0$	112
1	1		x				$x = y < 0 < s$, $-1 < z < y$	$ORTZ_1$	14	M_1	mC	110	$\bar{1}10$	001
	u		x	0			$x = y, z = 0$, $-u < x < 0$	LO_2	14	M_4	mC	110	$\bar{1}10$	001
	u		x				$x = y < 0 < s$, $-u < z < 0$	$LORZ_2$	14	M_1	mC	110	$\bar{1}10$	001
	u				0		$s = 0, -u < z$, $-u < y < x$	LRU_2	17	M_2	mC	$1\bar{1}0$	110	$\bar{1}0\bar{1}$
	1	0	0	0			$x = y = z = 0$	O_3	21	Q_3	tP	010	001	100
	1	-1	0	0			$x = -1$, $y = z = 0$	X_3	22	H	hP	010	001	100
	1		0	0			$y = z = 0$, $-1 < x < 0$	OX_3	23	O_5	oC	011	$01\bar{1}$	100
	1			y	0	u	$x = -1 + u/3$, $y = z = -2u/3$	T_3	24	R_1	hR	010	001	$\bar{1}\bar{1}\bar{1}$
1	1	0		y			$x = 0, y = z$, $-1 < y < 0$	OU_1	25	M_4	mC	011	$0\bar{1}1$	100
1	1			y			$y = z < x$, $x < 0 < s$	OTU_1	25	M_1	mC	011	$0\bar{1}1$	100
	1	0		y			$x = 0, y = z$, $-u < y < 0$	OU_3	25	M_4	mC	011	$0\bar{1}1$	100
	1			y	0		$y = z, s = 0$, $-u < y < -2u/3$	TV_3	25	M_1	mC	011	$0\bar{1}1$	100
	1			y			$-u < y = z < 0$, $-1 < x < 0 < s$	$OQUVX_3$	25	M_1	mC	011	$0\bar{1}1$	100
		0	0	0			$x = y = z = 0$	O_4	32	O_6	oP	100	010	001
		$-v$	0	0			$x = -v$, $y = z = 0$	X_4	40	O_5	oC	010	012	100
			0	0			$y = z = 0$, $-v < x < 0$	OX_4	35	M_6	mP	010	100	001
	u	0	$-u$	0			$x = z = 0$, $y = -u$	Y_2	36	O_5	oC	100	102	010
		0	$-u$	0			$x = z = 0$, $y = -u$	Y_4	36	O_5	oC	100	102	010
	u	0		0			$x = z = 0$, $-u < y < 0$	OY_2	33	M_6	mP	100	010	001
		0		0			$x = z = 0$, $-u < y < 0$	OY_4	33	M_6	mP	100	010	001

Table 4 (*cont.*)

		Determination												
u	v	x	y	z	s	w	Description	Genus	Ni	De	Br	Conv. cell		
	1	0	0	$-u$			$x=y=0$, $z=-u$	Z_3	38	O_5	oC	100	120	001
		0	0	$-u$			$x=y=0$, $z=-u$	Z_4	38	O_5	oC	100	120	001
	1	0	0				$x=y=0$, $-u<z<0$	OZ_3	34	M_6	mP	100	001	010
		0	0				$x=y=0$, $-u<z<0$	OZ_4	34	M_6	mP	100	001	010
		$-v$	$-u$	0			$x=-v$, $y=-u, z=0$	L_4	42	O_3	oI	100	010	112
		$-v$		0			$x=-v, z=0$, $-u<y<0$	LX_4	41	M_3	mC	012	$0\bar{1}0$	100
	u		$-u$	0			$y=-u, z=0$, $-u<x<0$	LY_2	37	M_3	mC	102	$\bar{1}00$	010
			$-u$	0			$y=-u, z=0$, $-v<x<0$	LY_4	37	M_3	mC	102	$\bar{1}00$	010
	1		0	$-u$			$y=0, z=-u$, $-1<x<0$	KZ_3	39	M_3	mC	120	100	001
			0	$-u$			$y=0, z=-u$, $-v<x<0$	KZ_4	39	M_3	mC	120	100	001
	1				0	u	$s=0$, $y+u=x+1$, $-u<z<-2u/3$	RT_3	43	M_1	mC	110	112	$\bar{1}00$
					0	u	$s=0$, $y+u=x+v$, $-u<z<0$	LR_4	43	M_1	mC	110	112	$\bar{1}00$
1	1	0					$x=0$, $-1<z<y<0$	OUZ_1	44	T_2	aP	100	010	001
1	1						$-1<z<y$, $y<x<0<s$	$ORTUZ_1$	44	T_1	aP	100	010	001
	u	0					$-u<y<x=0$, $-u<z<0$	$OUYZ_2$	44	T_2	aP	100	010	001
	u			0			$z=0$, $-u<y<x<0$	LOY_2	44	T_2	aP	100	010	001
	u						$-u<y<x<0$, $-u<z<0<s$	*	44	T_1	aP	100	010	001
	1	0					$x=0$, $-u<z<y<0$	OUZ_3	44	T_2	aP	100	010	001
	1		0				$-1<x<y=0$, $-u<z<0$	$KOXZ_3$	44	T_2	aP	100	010	001
	1				0		$s=0$, $y+u<x+1$, $-u<z<y$	RTV_3	44	T_1	aP	100	010	001
	1						$-1<x<0<s$, $-u<z<y<0$	†	44	T_1	aP	100	010	001
		0					$-u<y<x=0$, $-u<z<0$	$OUYZ_4$	44	T_2	aP	100	010	001
			0				$-v<x<y=0$, $-u<z<0$	$KOXZ_4$	44	T_2	aP	100	010	001
				0			$-v<x<z=0$, $-u<y<0$	$LOXY_4$	44	T_2	aP	100	010	001
					0		$s=0$, $y+u<x+v$, $-u<y, -u<z$	LRV_4	44	T_1	aP	100	010	001
							$-v<x<0<s$, $-u<y<0$, $-u<z<0$	‡	44	T_1	aP	100	010	001

* $LORUYZ_2$. † $KOQUVXZ_3$. ‡ $KLOUVXYZ_4$.

some other properties, especially those that are important for the given problem, it is welcome.*

* See the beginning of the section *Introduction*.

What does the division of lattices into genera look like from this point of view? If two lattices belong to the same genus they agree, of course, in the properties (i), (ii), (iii) from Definition 3. These properties, however,

Table 5. *Detailed relationships between particular divisions*

Notation: Br Bravais type; Ni Niggli lattice character; Ge genus; De Delaunay sort of symmetry.

Br	Ni	Ge	De					
cP	3	O_1			K_3			
cI	5	T_1	K_1					
cF	1	J_1		K_2				
hP	12	Z_1			H			
hP	12	Z_2			H			
hP	22	X_3			H			
hR	2	JO_1		R_2				
hR	4	OT_1	R_1					
hR	9	J_2		R_2				
hR	24	T_3	R_1					
tP	11	O_2			Q_3			
tP	21	O_3			Q_3			
tI	6	RT_1	Q_1					
tI	7	TU_1	Q_1					
tI	15	L_2		Q_2				
tI	18	F_1	Q_1					
tI	18	F_3	Q_1					
oP	32	O_4						O_6
oC	13	OZ_1					O_5	
oC	13	OZ_2					O_5	
oC	23	OX_3					O_5	
oC	36	Y_2					O_5	
oC	36	Y_4					O_5	
oC	38	Z_3					O_5	
oC	38	Z_4					O_5	
oC	40	X_4					O_5	
oI	8	RTU_1		O_2				
oI	19	FJ_1		O_2				
oI	19	FG_3		O_2				
oI	19	J_3			O_3			
oI	19	GJ_3			O_3			
oI	19	G_3				O_4		
oI	42	L_4			O_3			
oF	16	LR_2	O_1					
oF	26	F_2	O_1					
oF	26	F_4	O_1					
mP	33	OY_2						M_6
mP	33	OY_4						M_6
mP	34	OZ_3						M_6
mP	34	OZ_4						M_6
mP	35	OX_4						M_6
mC	10	$J\Psi_2$		M_2				
mC	10	$JO\Psi_2$		M_2				
mC	10	$J\Gamma_1$			M_3			
mC	10	$JO\Gamma_1$			M_3			
mC	10	$J\Gamma_2$			M_3			
mC	10	$JO\Gamma_2$			M_3			
mC	10	JO_2					M_5	
mC	14	$ORTZ_1$	M_1					
mC	14	$LORZ_2$	M_1					
mC	14	LO_2				M_4		
mC	17	LRU_2		M_2				
mC	20	$JO\Delta_1$		M_2				
mC	20	$GO\Delta_3$		M_2				
mC	20	$J\Sigma_3$			M_3			
mC	20	$GJO\Sigma_3$			M_3			
mC	20	GO_3					M_5	
mC	25	OTU_1	M_1					
mC	25	TV_3	M_1					
mC	25	$OQUVX_3$	M_1					
mC	25	OU_1				M_4		
mC	25	OU_3				M_4		
mC	27	FJ_2		M_2				
mC	27	FG_4		M_2				
mC	27	J_4			M_3			
mC	27	GJ_4			M_3			
mC	27	G_4					M_5	
mC	28	$F\Lambda_2$	M_1					
mC	28	$F\Lambda_4$	M_1					
mC	29	$F\Gamma_1$	M_1					
mC	29	$F\Gamma_2$	M_1					
mC	29	$F\Gamma_3$	M_1					
mC	29	$F\Gamma_4$	M_1					
mC	30	H_3	M_1					
mC	30	$H\Sigma_3$	M_1					
mC	30	H_4	M_1					
mC	30	$H\Sigma_4$	M_1					
mC	37	LY_2			M_3			
mC	37	LY_4			M_3			
mC	39	KZ_3			M_3			
mC	39	KZ_4			M_3			
mC	41	LX_4			M_3			
mC	43	RT_3	M_1					
mC	43	LR_4	M_1					
aP	31	$FJ\Gamma_1$	T_1					
aP	31	$JO\Gamma\Delta_1$	T_1					
aP	31	$FJ\Gamma_2$	T_1					
aP	31	$FJ\Lambda_2$	T_1					
aP	31	$J\Lambda\Psi_2$	T_1					
aP	31	*	T_1					
aP	31	HJ_3	T_1					
aP	31	$HJ\Sigma_3$	T_1					
aP	31	$FG\Gamma_3$	T_1					
aP	31	$GJ\Gamma\Theta_3$	T_1					
aP	31	†	T_1					
aP	31	HJ_4	T_1					
aP	31	$HJ\Sigma_4$	T_1					
aP	31	$J\Psi_4$	T_1					
aP	31	$J\Sigma\Psi_4$	T_1					
aP	31	$FG\Gamma_4$	T_1					
aP	31	$FG\Lambda_4$	T_1					
aP	31	$GJ\Gamma\Theta_4$	T_1					
aP	31	$GJ\Lambda\Psi_4$	T_1					
aP	31	‡	T_1					
aP	31	$J\Lambda_2$		T_2				
aP	31	$JO\Lambda_2$		T_2				
aP	31	$G\Gamma_3$		T_2				
aP	31	$GO\Gamma_3$		T_2				
aP	31	$G\Gamma_4$		T_2				
aP	31	$G\Lambda_4$		T_2				
aP	31	$J\Sigma_4$		T_2				
aP	31	§		T_2				
aP	31	GO_4			T_3			
aP	44	$ORTUZ_1$	T_1					
aP	44	$LORUYZ_2$	T_1					
aP	44	RTV_3	T_1					
aP	44	$KOQUVXZ_3$	T_1					
aP	44	LRV_4	T_1					
aP	44	$KLOUVXYZ_4$	T_1					
aP	44	OUZ_1		T_2				
aP	44	LOY_2		T_2				
aP	44	$OUYZ_2$		T_2				
aP	44	OUZ_3		T_2				
aP	44	$KOXZ_3$		T_2				
aP	44	$KOXZ_4$		T_2				
aP	44	$LOXY_4$		T_2				
aP	44	$OUYZ_4$		T_2				

* $JO\Lambda\Psi_2 \cup JO\Gamma\Delta\Lambda_2$. † $GO\Gamma\Delta_3 \cup GJO\Gamma\Theta\Sigma_3$. ‡ $GO\Gamma\Delta\Lambda_4 \cup GJO\Gamma\Theta\Sigma_4 \cup GJO\Lambda\Sigma\Psi_4$. § $GO\Gamma_4 \cup GO\Lambda_4 \cup GJO\Sigma_4$.

can hardly be considered important for crystallography. But with a more detailed analysis we can gradually discover that lattices of the same genus agree in a surprisingly great number of properties of crystallographic importance.

First, lattices of the same genus belong also to the same Delaunay sort, Niggli character and Bravais type. In this way, genera were constructed. However, the investigations that are now in progress show that lattices of the same genus also agree in the number of Buerger cells and in how many orientations these cells occur in the lattice. They further agree in the number of the densest directions and planes and in the symmetry of these planes. But even the formulae for the alternative Buerger cells and for the angles between the densest directions and planes are identical for all lattices of the same genus. The same can be said about the formulae giving the parameters of the conventional cell and the Delaunay quadruplets of vectors.

Thus, the genus appears to be a remarkably strong bond between lattices, much stronger than its definition seems to suggest. It is mainly this fact that in our opinion justifies the construction of the genus concept.

15. Proof

The idea of the proof is this. We define the genera according to Definition 3. We make no other assumptions concerning the properties of genera, we do not even know their number. No symbols are used for them, in particular not the symbols from the column 'Genus' in Tables 3 and 4. We use the concept of the Niggli image of a genus but do not know the description ('fundamental systems') of these Niggli images. The system of the Niggli images of all genera is denoted **N**. Obviously, the union of all sets of the system **N** is the set Π of all Niggli points. This is one side of the matter.

On the other side, we introduce formally and independently of the above concepts special subsets of E_5 called elementary regions. They are defined and denoted by means of Tables 3 and 4. Every entry of these tables determines an elementary region in the following way. In the column 'Genus', there is the symbol of the elementary region. The subscript of this symbol is called the index of this region. To the index there corresponds an inequality from (14). This inequality together with the inequalities from the column 'Description' then gives a full description of the elementary region.

[For example, the 61st entry of Table 3 defines the elementary region $FG\Lambda_4$. It is the set of points (3) that fulfil $z < y = u < v < 1$, $z/2 < x < z$.]

The three-dimensional intersections (u, v constant) of elementary regions can be seen in Figs. 1, 2, 3 and 4. According to what has just been said, there are altogether 127 elementary regions. They are purely geometrical objects in E_5 and have hitherto nothing in common with the genera. The set of all elementary regions is denoted **E**.

We verify the two following properties of elementary regions:

(i) Any two elementary regions are disjoint.

(ii) The union of all elementary regions is the set Π of all Niggli points.

This may be lengthy but can be done by simple manipulations with inequalities. The explicit description of the set Π follows from the conditions (8) and (9). Figs. 1, 2, 3 and 4 may prove useful. So much for elementary regions.

Now we put the two things together. The system **N** stands for a division of the set Π into non-overlapping classes. The system **E** stands for a division of the set Π into 127 non-overlapping classes. What interests us is the relation between the systems **N** and **E**. We prove the following two statements.

(iii) If the Niggli points of the lattices L_1, L_2 lie in the same elementary region then L_1, L_2 belong to the same genus.

(iv) If the Niggli points of the lattices L_1, L_2 lie in different elementary regions then L_1, L_2 belong to different genera.

This must be verified for any particular elementary region and any particular pair of these regions. It is the most tedious part of the paper but the calculations are straightforward and cause no difficulties. Again, Figs. 1, 2, 3 and 4 are of great help. From (iii) it follows that:

(v) Any elementary region is a part of the Niggli image of a genus.

And from (iv):

(vi) If E_1, E_2 are two different elementary regions, E_i being a part of the Niggli image of the genus G_i ($i = 1, 2$), then $G_1 \neq G_2$.

But the union of all elementary regions as well as the union of the Niggli images of all genera is the same set Π. This is possible only if each elementary region coincides with the Niggli image of a genus and the genera are in this way exhausted. This means that the systems **N** and **E** are identical.

In other words, the sets introduced in Tables 3 and 4 in the columns 'Genus'and 'Description'* stand for Niggli images of all genera. Knowing this, we can more or less easily prove any statement we have pronounced in the previous text.

16. Conclusions

Having first examined some ideas for solving the problem, we have eventually constructed a division of lattices into 127 classes called genera. They have open parameter ranges and form a subdivision of both the Niggli lattice characters and the Delaunay sorts of symmetry. The genus of a given lattice can be determined comfortably

* Completed by one of the inequalities in (14).

by means of an algorithm and a table. A suitable notation for the genera was introduced and their three-dimensional illustration found. The special feature of the division is a relatively great number of genera constituting the *mC* and *aP* lattices (43 in both cases). A detailed relationship between the Bravais types, Delaunay sorts, Niggli characters and genera was ascertained. The fact that lattices of the same genus have a fairly great number of crystallographically significant properties in common came as a welcome surprise.

APPENDIX *A*
How to find a Niggli point (Křivý & Gruber, 1976)

0. Choose an arbitrary primitive basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of the lattice L.
1. If $|\mathbf{a}| > |\mathbf{b}|$ or ($|\mathbf{a}| = |\mathbf{b}|$, $|\mathbf{b}\cdot\mathbf{c}| > |\mathbf{a}\cdot\mathbf{c}|$), change $\mathbf{a} \leftrightarrow \mathbf{b}$.
2. If $|\mathbf{b}| > |\mathbf{c}|$ or ($|\mathbf{b}| = |\mathbf{c}|$, $|\mathbf{a}\cdot\mathbf{c}| > |\mathbf{a}\cdot\mathbf{b}|$), change $\mathbf{b} \leftrightarrow \mathbf{c}$ and go to 1.
3. If neither $\mathbf{a}\cdot\mathbf{b} > 0$, $\mathbf{a}\cdot\mathbf{c} > 0$, $\mathbf{b}\cdot\mathbf{c} > 0$ nor $\mathbf{a}\cdot\mathbf{b} \leq 0$, $\mathbf{a}\cdot\mathbf{c} \leq 0$, $\mathbf{b}\cdot\mathbf{c} \leq 0$, change the sign of $\mathbf{a}$.
4. If neither $\mathbf{a}\cdot\mathbf{b} > 0$, $\mathbf{a}\cdot\mathbf{c} > 0$, $\mathbf{b}\cdot\mathbf{c} > 0$ nor $\mathbf{a}\cdot\mathbf{b} \leq 0$, $\mathbf{a}\cdot\mathbf{c} \leq 0$, $\mathbf{b}\cdot\mathbf{c} \leq 0$, change the sign of $\mathbf{b}$ and go to 3.
5. If $2|\mathbf{b}\cdot\mathbf{c}| > \mathbf{b}^2$ or ($2\mathbf{b}\cdot\mathbf{c} = \mathbf{b}^2$, $2\mathbf{a}\cdot\mathbf{c} < \mathbf{a}\cdot\mathbf{b}$) or ($2\mathbf{b}\cdot\mathbf{c} = -\mathbf{b}^2$, $\mathbf{a}\cdot\mathbf{b} < 0$), let $\mathbf{c} := \mathbf{c} - [\mathrm{sgn}(\mathbf{b}\cdot\mathbf{c})]\mathbf{b}$ and go to 1.
6. If $2|\mathbf{a}\cdot\mathbf{c}| > \mathbf{a}^2$ or ($2\mathbf{a}\cdot\mathbf{c} = \mathbf{a}^2$, $2\mathbf{b}\cdot\mathbf{c} < \mathbf{a}\cdot\mathbf{b}$) or ($2\mathbf{a}\cdot\mathbf{c} = -\mathbf{a}^2$, $\mathbf{a}\cdot\mathbf{b} < 0$), let $\mathbf{c} := \mathbf{c} - [\mathrm{sgn}(\mathbf{a}\cdot\mathbf{c})]\mathbf{a}$ and go to 1.
7. If $2|\mathbf{a}\cdot\mathbf{b}| > \mathbf{a}^2$ or ($2\mathbf{a}\cdot\mathbf{b} = \mathbf{a}^2$, $2\mathbf{b}\cdot\mathbf{c} < \mathbf{a}\cdot\mathbf{c}$) or ($2\mathbf{a}\cdot\mathbf{b} = -\mathbf{a}^2$, $\mathbf{a}\cdot\mathbf{c} < 0$), let $\mathbf{b} := \mathbf{b} - [\mathrm{sgn}(\mathbf{a}\cdot\mathbf{b})]\mathbf{a}$ and go to 1.
8. Let $K := \mathbf{a}^2 + \mathbf{b}^2 + 2\mathbf{a}\cdot\mathbf{b} + 2\mathbf{a}\cdot\mathbf{c} + 2\mathbf{b}\cdot\mathbf{c}$.
9. If $K < 0$ or ($K = 0$, $\mathbf{a}^2 + 2\mathbf{a}\cdot\mathbf{c} > \mathbf{b}^2 + 2\mathbf{b}\cdot\mathbf{c}$), let $\mathbf{c} := \mathbf{a} + \mathbf{b} + \mathbf{c}$ and go to 1.
10. Let $u := \mathbf{a}^2/\mathbf{c}^2$, $v := \mathbf{b}^2/\mathbf{c}^2$, $x := 2\mathbf{b}\cdot\mathbf{c}/\mathbf{c}^2$, $y := 2\mathbf{a}\cdot\mathbf{c}/\mathbf{c}^2$, $z := 2\mathbf{a}\cdot\mathbf{b}/\mathbf{c}^2$.

Then $[u, v, x, y, z]$ is the Niggli point of the lattice L.

APPENDIX *B*
How to determine all Buerger points of a lattice

A Buerger point is derived from a Buerger cell. Thus we have first to ascertain all Buerger cells of the given lattice L. These cells may be found according to Gruber (1973, 1989). Secondly, having a particular Buerger cell B of L, we have to find all Buerger points that follow from B. If (3) is such a Buerger point, then there exist vectors (1) that determine the cell B and fulfil (22). Any permutation of the vectors (1) as well as the change of sign of any of them determines also the cell B. In this way, we get a set of at most 24 points that contains (besides other points) all Buerger points of L that can be derived from the cell B. We have only to check the conditions (23) and (24). Special relations usually make it unnecessary to construct all the above 24 points.

APPENDIX *C*
How to find all Niggli bases of a lattice if one of them is known

First, they can be found in the *Comments* (Gruber, 1978*a*,*b*; Tables III*a*, *b*, *c*, *d*). If the *Comments* are not at hand, we take into consideration the fact that the transformation matrix between the given Niggli basis and another Niggli basis of the same lattice consists only of the numbers $-1, 0, 1$ (Gruber, 1970). This gives a finite number of possibilities. Again, special relations reduce the number of alternatives that are to be checked.

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