Table 3.1.3.2
Lattice characters described by relations between conventional cell parameters

Under each of the roman numerals below 'Lattice characters in', *numbers* of characters (*cf.* Table 3.1.3.1, first column) are listed for which the key parameter p lies in the interval defined by the same roman numeral below 'Intervals of p'. For instance, a lattice with character No. 15 under IV has $p = c/a$; so it falls in the interval IV with $2^{1/2} < c/a$ ($< \infty$); No. 33 under II has $p = b$; therefore the interval $a - c$ for II yields the relation $a < b < c$.

Lattice symmetry	Bravais type of lattice†	p = key parameter	Lattice characters in				Intervals of p					Conventions‡
			I	II	III	IV	I	II	III	IV		
Tetragonal	tP	c/a	21	11	–	–	0	1	∞	–	–	
Tetragonal	tI	c/a	18	6	7	15	0	$(2/3)^{1/2}$	1	$2^{1/2}$	∞	
Hexagonal	hP	c/a	22	12	–	–	0	1	∞	–	–	
Rhombohedral	hR	c/a	24	4	2	9	0	$(3/8)^{1/2}$	$(3/2)^{1/2}$	$6^{1/2}$	∞	Hexagonal axes
Orthorhombic	oP	–	32 no relations				–	–	–	–	–	$a < b < c$
Orthorhombic	oS											
$b < a\sqrt{3}$		c	23	13	–	–	0	d§	∞	–	–	$a < b$
$b > a\sqrt{3}$		c	40	36	38	–	0	a	d§	∞	–	
Orthorhombic	oI	r¶	8	19	42	–	0	a	b	∞	–	$a < b < c$
Orthorhombic	oF	b/a	16	26	–	–	1	$3^{1/2}$	∞	–	–	$a < b < c$
Monoclinic	mP	b	35	33	34	–	0	a	c	∞	–	$a < c$††
Monoclinic	mS											
Centred net = 1‡‡		b/a	–	–	–	28, 29						
Centred net = 2		b/a	–	–	–	30						
Centred net = 2, 3		b/a	37, 41	20	25	–	0	$(1/3)^{1/2}$	1	$3^{1/2}$	∞	C centred††
Centred net = 1, 2, 3		b/a	27, 39	10, 17	14	–						
Centred net = 3		b/a	43	–	–	–	1	∞	–	–	–	I centred††
Triclinic	aP	α, β, γ	31	44	–	–	60°	90°	120°	–	–	$a < b < c$
Cubic	cP	–		3	no relations		–	–	–	–	–	
	cI	–		5			–	–	–	–	–	
	cF	–		1			–	–	–	–	–	

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). ‡ These conventions refer to the cells obtained by the transformations of Table 3.1.3.1. They have been chosen for convenience in this table. § $d = \frac{1}{2}(a^2 + b^2)^{1/2}$. ¶ $r = \frac{1}{2}(a^2 + b^2 + c^2)^{1/2}$. †† Setting with unique axis b; $\beta > 90°$; $a < c$ for both P and I cells, $a < c$ or $a > c$ for C cells. ‡‡ This number specifies the centred net among the three orthogonal nets parallel to the twofold axis and passing through (1) the shortest, (2) the second shortest, and (3) the third shortest lattice vector perpendicular to the axis. For example, '2, 3' means that either net (2) or net (3) is the centred one.

It is impossible to perform a continuous deformation – within the centred orthogonal type – of an elongated net into a compressed one, since one has to pass through either a hexagonal or a quadratic net.

In three dimensions, lattices are of the same character if, first, a continuous deformation of one into the other is possible without leaving the Bravais type. Secondly, it is required that all matrix elements of the reduced form (3.1.3.1) change continuously during such a deformation. These criteria lead to 44 different *lattice characters* (Niggli, 1928; Buerger, 1957). Each of them can be recognized easily from the relations between the elements of the reduced form given in Table 3.1.3.1 [adapted from Table 5.1.3.1 in *International Tables for X-ray Crystallography* (1969), which was improved by Mighell & Rodgers (1980)]. The numbers in column 1 of this table are at the same time used as a general notation of the lattice characters themselves. We speak, for example, about the lattice character No. 7 (which is part of the Bravais type tI) *etc*.

In Table 3.1.3.2, another description of lattice characters is given by grouping together all characters of a given Bravais type and by indicating for each character the corresponding interval of values of a suitable parameter p, expressed in the usual parameters of a conventional cell. In systems where no generally accepted convention exists, the choice of this cell has been made for convenience in the last column of this table.

The subdistinctions 'centred net = 1, 2 or 3' for the monoclinic centred type are closely related to the description in other conventions. For instance, they correspond to C-, A- or I-centred cells, respectively, if **b** is the unique axis and **a** and **c** are the shortest vectors ($a < c$) perpendicular to **b**; note that in Table 3.1.3.2 only C and I, not A, cells are listed. From the multiple entries in Table 3.1.3.2 for this type, it follows that the description in terms of b/a is not exhaustive; the distinctions depend upon rather intricate relations (*cf.* Mighell *et al.*, 1975; Mighell & Rodgers, 1980).

No attempt has been made in Table 3.1.3.2 to specify whether the end points of p intervals are inclusive or not. For practical purposes, they can always be taken to be non-inclusive. Indeed, the end points correspond either to a different Bravais type or to a purely geometric singularity without physical significance. If p is very close to an interval limit of the latter kind, one should be aware of the fact that different measurements of such a lattice may yield different characters, with totally differing aspects of the reduced form.

3.1.3.6. Applications

Classification. The reduced basis can be used to derive the Bravais-lattice type and the conventional cell parameters, starting from an arbitrary description of the lattice. For this purpose, the reduced form is first derived from the given description, *e.g.* by means of the algorithm of Křivý & Gruber (1976). Subsequently it is compared with the reduced forms (Table 3.1.3.1) for the 44 lattice characters and transformed to the appropriate conventional cell. Thus the reduced cell is helpful as an accessory in classifications based on conventional cells.

Alternatively, the parameters of the reduced form itself (either of the direct lattice or of the reciprocal lattice) can be used as a basis for determinative classification.

Comparison of lattices. Two lattices, defined by their reduced cells, can be compared on a rigorous basis to find out whether they are identical lattices or are related by one cell being a subcell of the other (Santoro *et al.*, 1980).

Further properties of lattices are discussed in Section 3.1.4.

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3.1.4. Further properties of lattices

By B. Gruber and H. Grimmer

3.1.4.1. Further kinds of reduced cells

In Section 3.1.3.2, a 'reduced basis' of a lattice is defined which permits a unique representation of this lattice. It was introduced into crystallography by Niggli (1928) and incorporated into *International Tables for X-ray Crystallography* (1969), Vol. I. Originating from algebra (Eisenstein, 1851), a reduced basis is defined in a rather complicated manner [conditions (3.1.3.2*a*) to (3.1.3.5*f*) in Section 3.1.3.2] and lacks any geometrical meaning. A cell spanned by a reduced basis is called the *Niggli cell*.

However, unique primitive cells may be introduced also in other ways that – unlike the Niggli cell[3] – have significant geometrical features based mainly on extremal principles (Gruber, 1989). We shall describe some of them below.

If a (primitive) cell of the lattice **L** fulfils the condition

$$a + b + c = \min$$

on the set of all primitive cells of **L**, we call it a *Buerger cell*. This cell need not be unique with regard to its shape in the lattice. There exist lattices with 1, 2, 3, 4 and 5 (but not more) Buerger cells differing in shape. The uniqueness can be achieved by various additional conditions. In this way, we can arrive at the following four reduced cells:

(i) the Buerger cell with minimum surface;[4]
(ii) the Buerger cell with maximum surface;
(iii) the Buerger cell with minimum deviation;[5]
(iv) the Buerger cell with maximum deviation.

Equivalent definitions can be obtained by replacing the term 'surface' in (i) and (ii) by the expression

$$\sin\alpha + \sin\beta + \sin\gamma$$

or

$$\sin\alpha \sin\beta \sin\gamma,$$

and by replacing the 'deviation' in (iii) and (iv) by

$$|\cos\alpha| + |\cos\beta| + |\cos\gamma|$$

or

$$|\cos\alpha \cos\beta \cos\gamma|.$$

A Buerger cell can agree with more than one of the definitions

$$\text{(i), (ii), (iii), (iv).} \qquad (3.1.4.1)$$

[3] See, however, later parts of this section.
[4] Meaning that this cell has the smallest surface of all Buerger cells of the lattice.
[5] The deviation of a cell is the number $|90^\circ - \alpha| + |90^\circ - \beta| + |90^\circ - \gamma|$.

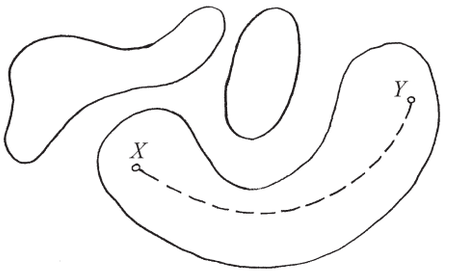

Figure 3.1.4.1
A set **M** in $\mathbb{E}^2$ consisting of three components.

For example, if a lattice has only one Buerger cell, then this cell agrees with all the definitions in (3.1.4.1). However, there exist also Buerger cells that are in agreement with none of them. Thus, the definitions (3.1.4.1) do not imply a partition of Buerger cells into classes.

It appears that case (iv) coincides with the Niggli cell. This is important because this cell can now be defined by a simple geometrical property instead of a complicated system of conditions.

Further reduced cells can be obtained by applying the definitions (3.1.4.1) to the reciprocal lattice. Then, to a Buerger cell in the reciprocal lattice, there corresponds a primitive cell with absolute minimum surface[6] in the direct lattice.

The reduced cells according to the definitions (3.1.4.1) can be recognized by means of a table and found in the lattice by means of algorithms. Detailed mutual relationships between them have been ascertained.

3.1.4.2. Topological characterization of lattice characters

In his thorough analysis of lattice characters, de Wolff (1988) remarks that so far they have not been defined as clearly as the Bravais types and that an exact general definition does not exist. Gruber (1992) tried to base such a definition on topological concepts.

The crucial notion is the decomposition of a set **M** of points of the n-dimensional Euclidean space $\mathbb{E}^n$ into equivalence classes called *components* of the set **M**. They can be defined as follows: Two points X, Y of the set **M** belong to the same component if they can be connected by a *continuous* path which lies entirely in the set **M** (Fig. 3.1.4.1). This partition of the set **M** into components is unique and is determined solely by the set **M**.

Now let us return to lattices. To any lattice **L** there is attached a point in $\mathbb{E}^5$ called the *Niggli point* of **L**. It is the point

$$\left[\frac{\mathbf{a}\cdot\mathbf{a}}{\mathbf{c}\cdot\mathbf{c}}, \frac{\mathbf{b}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{b}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}\right] \qquad (3.1.4.2)$$

provided that the vectors **a**, **b**, **c** describe the Niggli cell of **L** and fulfil the conditions (3.1.3.2*a*) to (3.1.3.5*f*) of Section 3.1.3.2. If $\mathscr{L}$ is a set of lattices then the set of Niggli points of all lattices of $\mathscr{L}$ is called the *Niggli image* of $\mathscr{L}$.

Thus we can speak about the Niggli image of a Bravais type $\mathscr{T}$. This Niggli image is a part of $\mathbb{E}^5$ and so can be partitioned into components. This division of Niggli points induces back a division of lattices of the Bravais type $\mathscr{T}$. It turns out that this division is identical with the division of $\mathscr{T}$ into lattice characters as introduced in Section 3.1.3.5. This fact, used conversely, can be considered an exact definition of the lattice characters: Two lattices of Bravais type $\mathscr{T}$ are said to be of the same lattice

[6] This cell need not be a Buerger cell.