Table 3.1.3.1
The parameters $D = \mathbf{b}\cdot\mathbf{c}$, $E = \mathbf{a}\cdot\mathbf{c}$ and $F = \mathbf{a}\cdot\mathbf{b}$ of the 44 lattice characters ($A = \mathbf{a}\cdot\mathbf{a}$, $B = \mathbf{b}\cdot\mathbf{b}$, $C = \mathbf{c}\cdot\mathbf{c}$)

The character of a lattice given by its reduced form (3.1.3.1) is the first one that agrees when the 44 entries are compared with that reduced form in the sequence given below (suggested by Gruber). Such a logical order is not always obeyed by the widely used character numbers (first column), which therefore show some reversals, *e.g.* 4 and 5.

No.	Type	D	E	F	Lattice symmetry	Bravais type of lattice†	Transformation to a conventional basis (*cf.* footnote ‡ to Table 3.1.3.2)
$A = B = C$							
1	I	$A/2$	$A/2$	$A/2$	Cubic	*cF*	$1\bar{1}1/11\bar{1}/\bar{1}11$
2	I	D	D	D	Rhombohedral	*hR*	$1\bar{1}0/101/\bar{1}\bar{1}1$
3	II	0	0	0	Cubic	*cP*	100/010/001
5	II	$-A/3$	$-A/3$	$-A/3$	Cubic	*cI*	101/110/011
4	II	D	D	D	Rhombohedral	*hR*	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}1$
6	II	D‡	D	F	Tetragonal	*tI*	011/101/110
7	II	D‡	E	E	Tetragonal	*tI*	101/110/011
8	II	D‡	E	F	Orthorhombic	*oI*	$\bar{1}\bar{1}0/\bar{1}01/0\bar{1}\bar{1}$
$A = B$, no conditions on C							
9	I	$A/2$	$A/2$	$A/2$	Rhombohedral	*hR*	$100/\bar{1}10/\bar{1}\bar{1}3$
10	I	D	D	F	Monoclinic	*mC*	$110/1\bar{1}0/00\bar{1}$
11	II	0	0	0	Tetragonal	*tP*	100/010/001
12	II	0	0	$-A/2$	Hexagonal	*hP*	100/010/001
13	II	0	0	F	Orthorhombic	*oC*	$110/\bar{1}10/001$
15	II	$-A/2$	$-A/2$	0	Tetragonal	*tI*	$\underline{1}00/0\underline{1}0/112$
16	II	D‡	D	F	Orthorhombic	*oF*	$\bar{1}\bar{1}0/\bar{1}10/112$
14	II	D	D	F	Monoclinic	*mC*	$110/\bar{1}10/001$
17	II	D‡	E	F	Monoclinic	*mC*	$1\bar{1}0/110/\bar{1}01$
$B = C$, no conditions on A							
18	I	$A/4$	$A/2$	$A/2$	Tetragonal	*tI*	$0\bar{1}1/1\bar{1}\bar{1}/100$
19	I	D	$A/2$	$A/2$	Orthorhombic	*oI*	$\bar{1}00/0\bar{1}1/\bar{1}11$
20	I	D	E	E	Monoclinic	*mC*	$011/01\bar{1}/100$
21	II	0	0	0	Tetragonal	*tP*	010/001/100
22	II	$-B/2$	0	0	Hexagonal	*hP*	010/001/100
23	II	D	0	0	Orthorhombic	*oC*	$011/0\bar{1}1/100$
24	II	D‡	$-A/3$	$-A/3$	Rhombohedral	*hR*	$121/0\bar{1}1/100$
25	II	D	E	E	Monoclinic	*mC*	$011/0\bar{1}1/100$
No conditions on A, B, C							
26	I	$A/4$	$A/2$	$A/2$	Orthorhombic	*oF*	$100/\bar{1}20/\bar{1}02$
27	I	D	$A/2$	$A/2$	Monoclinic	*mC*	$\bar{1}20/\bar{1}00/0\bar{1}1$
28	I	D	$A/2$	$2D$	Monoclinic	*mC*	$\bar{1}00/\bar{1}02/010$
29	I	D	$2D$	$A/2$	Monoclinic	*mC*	$100/1\bar{2}0/00\bar{1}$
30	I	$B/2$	E	$2E$	Monoclinic	*mC*	$010/012/\bar{1}00$
31	I	D	E	F	Triclinic	*aP*	100/010/001
32	II	0	0	0	Orthorhombic	*oP*	100/010/001
40	II	$-B/2$	0	0	Orthorhombic	*oC*	$0\bar{1}0/012/\bar{1}00$
35	II	D	0	0	Monoclinic	*mP*	$0\bar{1}0/\bar{1}00/00\bar{1}$
36	II	0	$-A/2$	0	Orthorhombic	*oC*	$100/\bar{1}02/010$
33	II	0	E	0	Monoclinic	*mP*	100/010/001
38	II	0	0	$-A/2$	Orthorhombic	*oC*	$\bar{1}00/120/00\bar{1}$
34	II	0	0	F	Monoclinic	*mP*	$\bar{1}00/00\bar{1}/0\bar{1}0$
42	II	$-B/2$	$-A/2$	0	Orthorhombic	*oI*	$\bar{1}00/0\bar{1}0/112$
41	II	$-B/2$	E	0	Monoclinic	*mC*	$0\bar{1}2/0\bar{1}0/\bar{1}00$
37	II	D	$-A/2$	0	Monoclinic	*mC*	$\underline{1}02/100/010$
39	II	D	0	$-A/2$	Monoclinic	*mC*	$\bar{1}\underline{2}0/\bar{1}\underline{0}0/00\bar{1}$
43	II	D§	E	F	Monoclinic	*mI*	$\bar{1}00/\bar{1}\underline{1}2/0\bar{1}0$
44	II	D	E	F	Triclinic	*aP*	100/010/001

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). The capital letter of the symbols in this column indicates the centring type of the cell as obtained by the transformation in the last column. For this reason, the standard symbols *mS* and *oS* are not used here. ‡ $2|D + E + F| = A + B$. § $2|D + E + F| = A + B$ plus $|2D + F| = B$.

with Fig. 3.1.3.3. This compressed type of centred orthogonal **a**, **b** net is limited by the case of a hexagonal net (where it merges with the elongated type, Fig. 3.1.3.4) and by the centred quadratic net (where it merges with the primitive orthogonal net, Fig. 3.1.3.2). In the limit of the hexagonal net, the triangle *Ohh* in Figs. 3.1.3.4 and 3.1.3.5 is all that remains, it is of type I except for the point *O*. For the quadratic net, only the type-II region in Fig. 3.1.3.5, then a triangle with all edges inclusive, is left. It corresponds to the triangle *Oqq* in Fig. 3.1.3.2.

3.1.3.5. Lattice characters

Apart from being unique, the reduced cell has the further advantage of allowing a much finer differentiation between types of lattices than is given by the Bravais types. For two-dimensional lattices, this is apparent already in the last section where the centred orthogonal class is subdivided into nets with elongated character and those with compressed character, depending on whether the shortest net vector is, or is not, a symmetry direction.

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 I	II	III	IV	Intervals of p I	II	III	IV		Conventions‡
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 or 29						
Centred net = 2		b/a	–	–	–	30						
Centred net = 2, 3		b/a	37 or 41	20	25	–	0	$(1/3)^{1/2}$	1	$3^{1/2}$	∞	*C* centred††
Centred net = 1, 2, 3		b/a	27 or 39	10 or 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.