

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

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	$\bar{1}\bar{1}\bar{1}/\bar{1}\bar{1}\bar{1}/\bar{1}\bar{1}\bar{1}$
2	I	D	D	D	Rhombohedral	hR	$\bar{1}\bar{1}\bar{0}/\bar{1}\bar{0}\bar{1}/\bar{1}\bar{1}\bar{1}$
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	$\bar{1}\bar{1}\bar{0}/\bar{1}\bar{0}\bar{1}/\bar{1}\bar{1}\bar{1}$
6	II	$D\ddagger$	D	F	Tetragonal	tI	011/101/110
7	II	$D\ddagger$	E	E	Tetragonal	tI	101/110/011
8	II	$D\ddagger$	E	F	Orthorhombic	oI	$\bar{1}\bar{1}\bar{0}/\bar{1}\bar{0}\bar{1}/\bar{0}\bar{1}\bar{1}$
$A = B$, no conditions on C							
9	I	$A/2$	$A/2$	$A/2$	Rhombohedral	hR	100/ $\bar{1}\bar{1}\bar{0}/\bar{1}\bar{1}\bar{3}$
10	I	D	D	F	Monoclinic	mC	110/ $\bar{1}\bar{1}\bar{0}/00\bar{1}$
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/ $\bar{1}\bar{1}\bar{0}/00\bar{1}$
15	II	$-A/2$	$-A/2$	0	Tetragonal	tI	100/010/112
16	II	$D\ddagger$	D	F	Orthorhombic	oF	$\bar{1}\bar{1}\bar{0}/\bar{1}\bar{1}\bar{0}/112$
14	II	D	D	F	Monoclinic	mC	110/ $\bar{1}\bar{1}\bar{0}/00\bar{1}$
17	II	$D\ddagger$	E	F	Monoclinic	mC	$\bar{1}\bar{1}\bar{0}/110/\bar{1}\bar{0}\bar{1}$
$B = C$, no conditions on A							
18	I	$A/4$	$A/2$	$A/2$	Tetragonal	tI	0 $\bar{1}\bar{1}$ / $\bar{1}\bar{1}\bar{1}/100$
19	I	D	$A/2$	$A/2$	Orthorhombic	oI	$\bar{1}\bar{0}\bar{0}/0\bar{1}\bar{1}/\bar{1}\bar{1}\bar{1}$
20	I	D	E	E	Monoclinic	mC	011/0 $\bar{1}\bar{1}/\bar{1}\bar{0}\bar{0}$
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 $\bar{1}\bar{1}/100$
24	II	$D\ddagger$	$-A/3$	$-A/3$	Rhombohedral	hR	121/0 $\bar{1}\bar{1}/100$
25	II	D	E	E	Monoclinic	mC	011/0 $\bar{1}\bar{1}/100$
No conditions on A, B, C							
26	I	$A/4$	$A/2$	$A/2$	Orthorhombic	oF	100/ $\bar{1}\bar{2}\bar{0}/\bar{1}\bar{0}\bar{2}$
27	I	D	$A/2$	$A/2$	Monoclinic	mC	$\bar{1}\bar{2}\bar{0}/\bar{1}\bar{0}\bar{0}/0\bar{1}\bar{1}$
28	I	D	$A/2$	$2D$	Monoclinic	mC	$\bar{1}\bar{0}\bar{0}/\bar{1}\bar{0}\bar{2}/010$
29	I	D	$2D$	$A/2$	Monoclinic	mC	100/ $\bar{1}\bar{2}\bar{0}/00\bar{1}$
30	I	$B/2$	E	$2E$	Monoclinic	mC	010/0 $\bar{1}\bar{2}/\bar{1}\bar{0}\bar{0}$
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 $\bar{1}\bar{0}/0\bar{1}\bar{2}/\bar{1}\bar{0}\bar{0}$
35	II	D	0	0	Monoclinic	mP	0 $\bar{1}\bar{0}/\bar{1}\bar{0}\bar{0}/00\bar{1}$
36	II	0	$-A/2$	0	Orthorhombic	oC	100/ $\bar{1}\bar{0}\bar{2}/010$
33	II	0	E	0	Monoclinic	mP	100/010/001
38	II	0	0	$-A/2$	Orthorhombic	oC	$\bar{1}\bar{0}\bar{0}/1\bar{2}\bar{0}/00\bar{1}$
34	II	0	0	F	Monoclinic	mP	$\bar{1}\bar{0}\bar{0}/0\bar{0}\bar{1}/0\bar{1}\bar{0}$
42	II	$-B/2$	$-A/2$	0	Orthorhombic	oI	$\bar{1}\bar{0}\bar{0}/0\bar{1}\bar{0}/112$
41	II	$-B/2$	E	0	Monoclinic	mC	0 $\bar{1}\bar{2}/0\bar{1}\bar{0}/\bar{1}\bar{0}\bar{0}$
37	II	D	$-A/2$	0	Monoclinic	mC	102/ $\bar{1}\bar{0}\bar{0}/010$
39	II	D	0	$-A/2$	Monoclinic	mC	$\bar{1}\bar{2}\bar{0}/\bar{1}\bar{0}\bar{0}/00\bar{1}$
43	II	$D\§$	E	F	Monoclinic	mI	100/ $\bar{1}\bar{1}\bar{2}/0\bar{1}\bar{0}$
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 \mathbf{a}, \mathbf{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.