1.2. Application to the crystal systems

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Information on the description and classification of Bravais lattices, their assignment to crystal systems, the choice of basis vectors for reduced or conventional basis systems, and on basis transformations is given in *IT* A (1983, Parts 5 and 9). In the following, for each crystal system, the metrical conditions for conventionally chosen basis systems and the possible Bravais types of lattices are listed. As some of the general formulae from Chapter 1.1 become simpler when not applied to a lattice with general (triclinic) metric, these simplified formulae are tabulated for all crystal systems (except triclinic).

Except for triclinic, monoclinic, and orthorhombic symmetry, tables are given that relate pairs h, k or triplets h, k, l of indices to certain sums s of products of these indices needed in equation (1.1.2.2). Such tables may be useful, for example, for indexing powder diffraction patterns.

1.2.1. Triclinic crystal system

No metrical conditions:	$a, b, c, \alpha, \beta, \gamma$ arbitrary
Bravais lattice type:	*aP*
Symmetry of lattice points:	$\bar{1}$

1.2.2. Monoclinic crystal system

Bravais lattice types:	*mP*, *mS*
Symmetry of lattice points	$2/m$

1.2.2.1. *Setting with 'unique axis* **b**'

Metrical conditions:	a, b, c, β arbitrary; $\alpha = \gamma = 90^\circ$
Bravais lattice types:	*mP*, *mC* or *mA* or *mI*
Symmetry of lattice points:	$.2/m.$

Simplified formulae:

$$V = (\mathbf{abc}) = \left[\begin{vmatrix} a^2 & 0 & ac\cos\beta \\ 0 & b^2 & 0 \\ ac\cos\beta & 0 & c^2 \end{vmatrix}\right]^{1/2} = abc\sin\beta, \qquad (1.1.1.1a)$$

$$\left.\begin{array}{l} a^* = \dfrac{1}{a\sin\beta}, \quad b^* = \dfrac{1}{b}, \quad c^* = \dfrac{1}{c\sin\beta}, \\ \alpha^* = \gamma^* = 90^\circ, \quad \beta^* = 180^\circ - \beta, \end{array}\right\} \qquad (1.1.1.3a)$$

$$V^* = (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \left[\begin{vmatrix} a^{*2} & 0 & a^*c^*\cos\beta^* \\ 0 & b^{*2} & 0 \\ a^*c^*\cos\beta^* & 0 & c^{*2} \end{vmatrix}\right]^{1/2} = a^*b^*c^*\sin\beta^*, \qquad (1.1.1.4a)$$

$$\left.\begin{array}{l} a = \dfrac{1}{a^*\sin\beta^*}, \quad b = \dfrac{1}{b^*}, \quad c = \dfrac{1}{c^*\sin\beta^*}, \\ \alpha = \gamma = 90^\circ, \quad \beta = 180^\circ - \beta^*, \end{array}\right\} \qquad (1.1.1.7a)$$

$$t^2 = u^2a^2 + v^2b^2 + w^2c^2 + 2uwac\cos\beta, \qquad (1.1.2.1a)$$

$$r^{*2} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hla^*c^*\cos\beta^*, \qquad (1.1.2.2a)$$

$$\frac{a}{h}(au + cw\cos\beta) = \frac{b^2v}{k} = \frac{c}{l}(au\cos\beta + cw), \qquad (1.1.2.12a)$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 = u_1u_2a^2 + v_1v_2b^2 + w_1w_2c^2 + (u_1w_2 + u_2w_1)ac\cos\beta, \qquad (1.1.3.4a)$$

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = h_1h_2a^{*2} + k_1k_2b^{*2} + l_1l_2c^{*2} + (h_1l_2 + h_2l_1)a^*c^*\cos\beta^*. \qquad (1.1.3.7a)$$

1.2.2.2. *Setting with 'unique axis* **c**'

Metrical conditions:	a, b, c, γ arbitrary; $\alpha = \beta = 90^\circ$
Bravais lattice types:	*mP*, *mB* or *mA* or *mI*
Symmetry of lattice points:	$..2/m$

Simplified formulae:

$$V = (\mathbf{abc}) = \left[\begin{vmatrix} a^2 & ab\cos\gamma & 0 \\ ab\cos\gamma & b^2 & 0 \\ 0 & 0 & c^2 \end{vmatrix}\right]^{1/2} = abc\sin\gamma, \qquad (1.1.1.1b)$$

$$\left.\begin{array}{l} a^* = \dfrac{1}{a\sin\gamma}, \quad b^* = \dfrac{1}{b\sin\gamma}, \quad c^* = \dfrac{1}{c}, \\ \alpha^* = \beta^* = 90^\circ, \quad \gamma^* = 180^\circ - \gamma, \end{array}\right\} \qquad (1.1.1.3b)$$

$$V^* = (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \left[\begin{vmatrix} a^{*2} & a^*b^*\cos\gamma^* & 0 \\ a^*b^*\cos\gamma^* & b^{*2} & 0 \\ 0 & 0 & c^{*2} \end{vmatrix}\right]^{1/2} = a^*b^*c^*\sin\gamma^*, \qquad (1.1.1.4b)$$

$$\left.\begin{array}{l} a = \dfrac{1}{a^*\sin\gamma^*}, \quad b = \dfrac{1}{b^*\sin\gamma^*}, \quad c = \dfrac{1}{c^*}, \\ \alpha = \beta = 90^\circ, \quad \gamma = 180^\circ - \gamma^*, \end{array}\right\} \qquad (1.1.1.7b)$$

$$t^2 = u^2a^2 + v^2b^2 + w^2c^2 + 2uvab\cos\gamma, \qquad (1.1.2.1b)$$

$$r^{*2} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hka^*b^*\cos\gamma^*, \qquad (1.1.2.2b)$$

$$\frac{a}{h}(au + bv\cos\gamma) = \frac{b}{k}(au\cos\gamma + bv) = \frac{c^2w}{l}, \qquad (1.1.2.12b)$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 = u_1u_2a^2 + v_1v_2b^2 + w_1w_2c^2 + (u_1v_2 + u_2v_1)ab\cos\gamma, \qquad (1.1.3.4b)$$

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = h_1h_2a^{*2} + k_1k_2b^{*2} + l_1l_2c^{*2} + (h_1k_2 + h_2k_1)a^*b^*\cos\gamma^*. \qquad (1.1.3.7b)$$

1.2.3. Orthorhombic crystal system

Metrical conditions:	a, b, c arbitrary; $\alpha = \beta = \gamma = 90^\circ$
Bravais lattice types:	*oP*, *oS* (*oC*, *oA*), *oI*, *oF*
Symmetry of lattice points:	*mmm*

Simplified formulae:

$$V = (\mathbf{abc}) = \left[\begin{vmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{vmatrix}\right]^{1/2} = abc, \qquad (1.1.1.1c)$$

$$a^* = \frac{1}{a}, \quad b^* = \frac{1}{b}, \quad c^* = \frac{1}{c}, \quad \alpha^* = \beta^* = \gamma^* = 90^\circ, \qquad (1.1.1.3c)$$

$$V^* = (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \left[\begin{vmatrix} a^{*2} & 0 & 0 \\ 0 & b^{*2} & 0 \\ 0 & 0 & c^{*2} \end{vmatrix}\right]^{1/2}$$
$$= a^*b^*c^* = a^{-1}b^{-1}c^{-1}, \qquad (1.1.1.4c)$$

$$a = \frac{1}{a^*}, \quad b = \frac{1}{b^*}, \quad c = \frac{1}{c^*}, \quad \alpha = \beta = \gamma = 90^\circ, \qquad (1.1.1.7c)$$

$$t^2 = u^2a^2 + v^2b^2 + w^2c^2, \qquad (1.1.2.1c)$$

$$r^{*2} = h^2a^{*2} + k^2b^{*2} + l^2w^{*2}, \qquad (1.1.2.2c)$$

$$\frac{a^2u}{h} = \frac{b^2v}{k} = \frac{c^2w}{l}, \qquad (1.1.2.12c)$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 = u_1u_2a^2 + v_1v_2b^2 + w_1w_2c^2, \qquad (1.1.3.4c)$$

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = h_1h_2a^{*2} + k_1k_2b^{*2} + l_1l_2c^{*2}. \qquad (1.1.3.7c)$$

1.2.4. Tetragonal crystal system

Metrical conditions: $a = b$; c arbitrary; $\alpha = \beta = \gamma = 90^\circ$
Bravais lattice types: tP, tI
Symmetry of lattice points: $4/mmm$
Simplified formulae:

$$V = (\mathbf{abc}) = \left[\begin{vmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & c^2 \end{vmatrix}\right]^{1/2} = a^2c, \qquad (1.1.1.1d)$$

$$a^* = b^* = \frac{1}{a}, \quad c^* = \frac{1}{c}, \quad \alpha^* = \beta^* = \gamma^* = 90^\circ, \qquad (1.1.1.3d)$$

$$V^* = (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \left[\begin{vmatrix} a^{*2} & 0 & 0 \\ 0 & a^{*2} & 0 \\ 0 & 0 & c^{*2} \end{vmatrix}\right]^{1/2}$$
$$= a^{*2}c^* = a^{-2}c^{-1}, \qquad (1.1.1.4d)$$

$$a = b = \frac{1}{a^*}, \quad c = \frac{1}{c^*}, \quad \alpha = \beta = \gamma = 90^\circ, \qquad (1.1.1.7d)$$

$$t^2 = (u^2 + v^2)a^2 + w^2c^2, \qquad (1.1.2.1d)$$

$$r^{*2} = (h^2 + k^2)a^{*2} + l^2c^{*2} = sa^{*2} + l^2c^{*2} \qquad (1.1.2.2d)$$

with

$$s = h^2 + k^2.$$

For each value of $s \leq 100$, all corresponding pairs h, k are listed in Table 1.2.4.1.

Table 1.2.4.1. *Assignment of integers $s \leq 100$ to pairs h, k with $s = h^2 + k^2$*

Each pair h, k represents all eight pairs which result from permutation and different sign combinations.

s	$h\ k$	s	$h\ k$	s	$h\ k$
1	1 0	32	4 4	68	8 2
2	1 1	34	5 3	72	6 6
4	2 0	36	6 0	73	8 3
5	2 1	37	6 1	74	7 5
8	2 2	40	6 2	80	8 4
9	3 0	41	5 4	81	9 0
10	3 1	45	6 3	82	9 1
13	3 2	49	7 0	85	9 2
16	4 0	50	7 1		7 6
17	4 1		5 5	89	8 5
18	3 3	52	6 4	90	9 3
20	4 2	53	7 2	97	9 4
25	5 0	58	7 3	98	7 7
	4 3	61	6 5	100	10 0
26	5 1	64	8 0		8 6
29	5 2	65	8 1		
			7 4		

$$\frac{u}{h} = \frac{v}{k} = \frac{c^2w}{a^2l}, \qquad (1.1.2.12d)$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 = (u_1u_2 + v_1v_2)a^2 + w_1w_2c^2, \qquad (1.1.3.4d)$$

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = (h_1h_2 + k_1k_2)a^{*2} + l_1l_2c^{*2}. \qquad (1.1.3.7d)$$

1.2.5. Trigonal and hexagonal crystal system

1.2.5.1. *Description referred to hexagonal axes*

Metrical conditions: $a = b$; c arbitrary; $\alpha = \beta = 90^\circ$; $\gamma = 120^\circ$
Bravais lattice types: hP, hR
Symmetry of lattice points: $6/mmm$ (hP), $\bar{3}m$ (hR)
Simplified formulae:

$$V = (\mathbf{abc}) = \left[\begin{vmatrix} a^2 & -\frac{1}{2}a^2 & 0 \\ -\frac{1}{2}a^2 & a^2 & 0 \\ 0 & 0 & c^2 \end{vmatrix}\right]^{1/2} = \tfrac{1}{2}\sqrt{3}\,a^2c, \qquad (1.1.1.1e)$$

$$\left.\begin{array}{l} a^* = b^* = \frac{2}{3}\sqrt{3}\frac{1}{a}, \quad c^* = \frac{1}{c}, \\ \alpha^* = \beta^* = 90^\circ, \quad \gamma^* = 60^\circ, \end{array}\right\} \qquad (1.1.1.3e)$$

$$V^* = (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \left[\begin{vmatrix} a^{*2} & \frac{1}{2}a^{*2} & 0 \\ \frac{1}{2}a^{*2} & a^{*2} & 0 \\ 0 & 0 & c^{*2} \end{vmatrix}\right]^{1/2}$$
$$= \tfrac{1}{2}\sqrt{3}\,a^{*2}c^* = \tfrac{2}{3}\sqrt{3}\,a^{-2}c^{-1}, \qquad (1.1.1.4e)$$

$$a = b = \tfrac{2}{3}\sqrt{3}\frac{1}{a^*}, \quad c = \frac{1}{c^*}, \quad \alpha = \beta = 90^\circ, \quad \gamma = 120^\circ, \qquad (1.1.1.7e)$$

$$t^2 = (u^2 + v^2 - uv)a^2 + w^2c^2, \qquad (1.1.2.1e)$$

$$r^{*2} = (h^2 + k^2 + hk)a^{*2} + l^2c^{*2} = sa^{*2} + l^2c^{*2} \qquad (1.1.2.2e)$$

with

Table 1.2.5.1. *Assignment of integers $s \leq 100$ to pairs h, k with* $s = h^2 + k^2 + hk$

Each pair h, k represents in addition the pairs $k, -h-k$ and $-h-k, h$, the permutations of these three, and the six corresponding centrosymmetrical pairs.

s	h k	s	h k	s	h k
1	1 0	31	5 1	67	7 2
3	1 1	36	6 0	73	8 1
4	2 0	37	4 3	75	5 5
7	2 1	39	5 2	76	6 4
9	3 0	43	6 1	79	7 3
12	2 2	48	4 4	81	9 0
13	3 1	49	7 0	84	8 2
16	4 0		5 3	91	9 1
19	3 2	52	6 2		6 5
21	4 1	57	7 1	93	7 4
25	5 0	61	5 4	97	8 3
27	3 3	63	6 3	100	10 0
28	4 2	64	8 0		

$$s = h^2 + k^2 + hk.$$

For each value of $s \leq 100$, all corresponding pairs h, k are listed in Table 1.2.5.1.

$$\frac{2u - v}{2h} = \frac{2v - u}{2k} = \frac{c^2 w}{a^2 l}, \qquad (1.1.2.12e)$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 = (u_1 u_2 + v_1 v_2 - \tfrac{1}{2} u_1 v_2 - \tfrac{1}{2} u_2 v_1) a^2 + w_1 w_2 c^2, \quad (1.1.3.4e)$$

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = (h_1 h_2 + k_1 k_2 + \tfrac{1}{2} h_1 k_2 + \tfrac{1}{2} h_2 k_1) a^{*2} + l_1 l_2 c^{*2}. \quad (1.1.3.7e)$$

1.2.5.2. *Description referred to rhombohedral axes*

Metrical conditions: $a = b = c; \alpha = \beta = \gamma$
Bravais lattice type: hR
Symmetry of lattice points: $\bar{3}m$
Simplified formulae:

$$V = (\mathbf{abc}) = \left[\begin{vmatrix} a^2 & a^2 \cos\alpha & a^2 \cos\alpha \\ a^2 \cos\alpha & a^2 & a^2 \cos\alpha \\ a^2 \cos\alpha & a^2 \cos\alpha & a^2 \end{vmatrix} \right]^{1/2}$$

$$= a^3 [1 - 3\cos^2\alpha + 2\cos^3\alpha]^{1/2}$$

$$= 2a^3 \left[\sin\tfrac{3}{2}\alpha \sin^3 \frac{\alpha}{2} \right]^{1/2}, \qquad (1.1.1.1f)$$

$$\left. \begin{aligned} \cos\frac{\alpha^*}{2} = \cos\frac{\beta^*}{2} = \cos\frac{\gamma^*}{2} = \frac{1}{2\cos\alpha/2}, \\ a^* = b^* = c^* = \frac{1}{a \sin\alpha \sin\alpha^*}, \end{aligned} \right\} \qquad (1.1.1.3f)$$

$$V^* = (\mathbf{a}^* \mathbf{b}^* \mathbf{c}^*)$$

$$= \left[\begin{vmatrix} a^{*2} & a^{*2} \cos\alpha^* & a^{*2} \cos\alpha^* \\ a^{*2} \cos\alpha^* & a^{*2} & a^{*2} \cos\alpha^* \\ a^{*2} \cos\alpha^* & a^{*2} \cos\alpha^* & a^{*2} \end{vmatrix} \right]^{1/2}$$

$$= a^{*3} [1 - 3\cos^2\alpha^* + 2\cos^3\alpha^*]^{1/2}$$

$$= 2a^{*3} \left[\sin\tfrac{3}{2}\alpha^* \sin^3 \frac{\alpha^*}{2} \right]^{1/2}, \qquad (1.1.1.4f)$$

Table 1.2.5.2. *Asssignment of integers $s_1 \leq 50$ to triplets h, k, l with $s_1 = h^2 + k^2 + l^2$ and to integers $s_2 = hk + hl + kl$*

Each triplet h, k, l represents all twelve triplets resulting from permutation and/or simultaneous change of all signs.

s_1	s_2	h	k	l	s_1	s_2	h	k	l	s_1	s_2	h	k	l
1	0	1	0	0	24	−12	−4	2	2	38	−19	−5	3	2
2	−1	−1	1	0		−4	4	−2	2		−11	−6	1	1
	1	1	1	0		20	4	2	2			5	−3	2
3	−1	−1	1	1	25	−12	−4	3	0		−1	6	−1	1
	3	1	1	1		0	5	0	0			5	3	−2
4	0	2	0	0		12	4	3	0		13	6	1	1
5	−2	−2	1	0	26	−13	−4	3	1		31	5	3	2
	2	2	1	0		−11	4	−3	1	40	−12	−6	2	0
6	−3	−2	1	1		−5	−5	1	0		12	6	2	0
	−1	2	−1	1		5	5	1	0	41	−20	−5	4	0
	5	2	1	1			4	3	−1		−16	−6	2	1
8	−4	−2	2	0		19	4	3	1			−4	4	3
	4	2	2	0	27	−9	−5	1	1		−8	6	−2	1
9	−4	−2	2	1			−3	3	3			4	4	−3
	0	3	0	0		−1	5	−1	1		4	6	2	−1
		2	2	−1		11	5	1	1		20	6	2	1
	8	2	2	1		27	3	3	3			5	4	0
10	−3	−3	1	0	29	−14	−4	3	2		40	4	4	3
	3	3	1	0		−10	−5	2	0	42	−21	−5	4	1
11	−5	−3	1	1			4	−3	2		−19	5	−4	1
	−1	3	−1	1		−2	4	3	−2		11	5	4	−1
	7	3	1	1		10	5	2	0		29	5	4	1
12	−4	−2	2	2		26	4	3	2	43	−21	−5	3	3
	12	2	2	2	30	−13	−5	2	1		−9	5	−3	3
13	−6	−3	2	0		−7	5	−2	1		39	5	3	3
	6	3	2	0		3	5	2	−1	44	−20	−6	2	2
14	−7	−3	2	1		17	5	2	1		−4	6	−2	2
	−5	3	−2	1	32	−16	−4	4	0		28	6	2	2
	1	3	2	−1		16	4	4	0	45	−22	−5	4	2
	11	3	2	1	33	−16	−5	2	2		−18	−6	3	0
16	0	4	0	0			−4	4	1			5	−4	2
17	−8	−3	2	2		−4	5	−2	2		2	5	4	−2
	−4	−4	1	0		8	4	4	−1		18	6	3	0
		3	−2	2		24	5	2	2		38	5	4	2
	4	4	1	0			4	4	1	46	−21	−6	3	1
	16	3	2	2	34	−15	−5	3	0		−15	6	−3	1
18	−9	−3	3	0			−4	3	3		9	6	3	−1
	−7	−4	1	1		−9	4	−3	3		27	6	3	1
	−1	4	−1	1		15	5	3	0	48	−16	−4	4	4
	9	4	1	1		33	4	3	3		48	4	4	4
		3	3	0	35	−17	−5	3	1	49	−24	−6	3	2
19	−9	−3	3	1		−13	5	−3	1		−12	6	−3	2
	3	3	3	−1		7	5	3	−1		0	7	0	0
	15	3	3	1		23	5	3	1			6	3	−2
20	−8	−4	2	0	36	−16	−4	4	2		36	6	3	2
	8	4	2	0		0	6	0	0	50	−25	−5	5	0
21	−10	−4	2	1			4	4	−2		−23	−5	4	3
	−6	4	−2	1		32	4	4	2		−17	5	−4	3
	2	4	2	−1	37	−6	−6	1	0		−7	−7	1	0
	14	4	2	1		6	6	1	0			5	4	−3
22	−9	−3	3	2							7	7	1	0
	−3	3	3	−2							25	5	5	0
	21	3	3	2							47	5	4	3

$$\left. \begin{aligned} \cos\frac{\alpha}{2} = \cos\frac{\beta}{2} = \cos\frac{\gamma}{2} = \frac{1}{2\cos\alpha^*/2}, \\ a = b = c = \frac{1}{a^* \sin\alpha^* \sin\alpha}, \end{aligned} \right\} \qquad (1.1.1.7f)$$

$$t^2 = (u^2 + v^2 + w^2) a^2 + 2(uv + uw + vw) a^2 \cos\alpha, \quad (1.1.2.1f)$$

$$r^{*2} = (h^2 + k^2 + l^2)a^{*2} + 2(hk + hl + kl)a^{*2}\cos\alpha^* = s_1 a^{*2} + 2s_2 a^{*2}\cos\alpha^* \quad (1.1.2.2f)$$

with

$$s_1 = h^2 + k^2 + l^2 \quad \text{and} \quad s_2 = hk + hl + kl.$$

For each value of $s_1 \leq 50$, all corresponding values of s_2 and all triplets h, k, l are listed in Table 1.2.5.2.

$$\frac{u}{h} + \frac{v+w}{h}\cos\alpha = \frac{v}{k} + \frac{u+w}{k}\cos\alpha = \frac{w}{l} + \frac{u+v}{l}\cos\alpha, \quad (1.1.2.12f)$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 = (u_1u_2 + v_1v_2 + w_1w_2)a^2 + (u_1v_2 + u_2v_1 + u_1w_2 + u_2w_1 + v_1w_2 + v_2w_1)a^2\cos\alpha, \quad (1.1.3.4f)$$

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = (h_1h_2 + k_1k_2 + l_1l_2)a^{*2} + (h_1k_2 + h_2k_1 + h_1l_2 + h_2l_1 + k_1l_2 + k_2l_1)a^{*2}\cos\alpha^*. \quad (1.1.3.7f)$$

1.2.6. Cubic crystal system

Metrical conditions:	$a = b = c$; $\alpha = \beta = \gamma = 90^\circ$
Bravais lattice types:	cP, cI, cF
Symmetry of lattice points:	$m\bar{3}m$

Simplified formulae:

$$V = (\mathbf{abc}) = \left[\begin{vmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & a^2 \end{vmatrix}\right]^{1/2} = a^3, \quad (1.1.1.1g)$$

$$a^* = b^* = c^* = \frac{1}{a}, \quad \alpha^* = \beta^* = \gamma^* = 90^\circ, \quad (1.1.1.3g)$$

$$V^* = (\mathbf{a}^*\mathbf{b}^*\mathbf{c}^*) = \left[\begin{vmatrix} a^{*2} & 0 & 0 \\ 0 & a^{*2} & 0 \\ 0 & 0 & a^{*2} \end{vmatrix}\right]^{1/2} = a^{*3} = a^{-3}, \quad (1.1.1.4g)$$

$$a = b = c = \frac{1}{a^*}, \quad \alpha = \beta = \gamma = 90^\circ, \quad (1.1.1.7g)$$

$$t^2 = (u^2 + v^2 + w^2)a^2, \quad (1.1.2.1g)$$

$$r^{*2} = (h^2 + k^2 + l^2)a^{*2} = sa^{*2} \quad (1.1.2.2g)$$

with

$$s = h^2 + k^2 + l^2.$$

For each value of $s \leq 100$, all corresponding triplets h, k, l are listed in Table 1.2.6.1.

$$\frac{u}{h} = \frac{v}{k} = \frac{w}{l}, \quad (1.1.2.12g)$$

$$\mathbf{t}_1 \cdot \mathbf{t}_2 = (u_1u_2 + v_1v_2 + w_1w_2)a^2, \quad (1.1.3.4g)$$

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = (h_1h_2 + k_1k_2 + l_1l_2)a^{*2}. \quad (1.1.3.7g)$$

Table 1.2.6.1. *Assignment of integers $s \leq 100$ to triplets h, k, l with $s = h^2 + k^2 + l^2$*

Each triplet represents all 48 triplets resulting from permutations and sign combinations.

s	*h k l*	*s*	*h k l*	*s*	*h k l*	*s*	*h k l*	*s*	*h k l*	*s*	*h k l*
1	1 0 0	25	5 0 0	42	5 4 1	59	7 3 1	74	8 3 1	88	6 6 4
2	1 1 0		4 3 0	43	5 3 3		5 5 3		7 5 0	89	9 2 2
3	1 1 1	26	5 1 0	44	6 2 2	61	6 5 0		7 4 3		8 5 0
4	2 0 0		4 3 1	45	6 3 0		6 4 3	75	7 5 1		8 4 3
5	2 1 0	27	5 1 1		5 4 2	62	7 3 2		5 5 5		7 6 2
6	2 1 1		3 3 3	46	6 3 1		6 5 1	76	6 6 2	90	9 3 0
8	2 2 0	29	5 2 0	48	4 4 4	64	8 0 0	77	8 3 2		8 5 1
9	3 0 0		4 3 2	49	7 0 0	65	8 1 0		6 5 4		7 5 4
	2 2 1	30	5 2 1		6 3 2		7 4 0	78	7 5 2	91	9 3 1
10	3 1 0	32	4 4 0	50	7 1 0		6 5 2	80	8 4 0	93	8 5 2
11	3 1 1	33	5 2 2		5 5 0	66	8 1 1	81	9 0 0	94	9 3 2
12	2 2 2		4 4 1		5 4 3		7 4 1		8 4 1		7 6 3
13	3 2 0	34	5 3 0	51	7 1 1		5 5 4		7 4 4	96	8 4 4
14	3 2 1		4 3 3		5 5 1	67	7 3 3		6 6 3	97	9 4 0
16	4 0 0	35	5 3 1	52	6 4 0	68	8 2 0	82	9 1 0		6 6 5
17	4 1 0	36	6 0 0	53	7 2 0		6 4 4		8 3 3	98	9 4 1
	3 2 2		4 4 2		6 4 1	69	8 2 1	83	9 1 1		8 5 3
18	4 1 1	37	6 1 0	54	7 2 1		7 4 2		7 5 3		7 7 0
	3 3 0	38	6 1 1		6 3 3	70	6 5 3	84	8 4 2	99	9 3 3
19	3 3 1		5 3 2		5 5 2	72	8 2 2	85	9 2 0		7 7 1
20	4 2 0	40	6 2 0	56	6 4 2		6 6 0		7 6 0		7 5 5
21	4 2 1	41	6 2 1	57	7 2 2	73	8 3 0	86	9 2 1	100	10 0 0
22	3 3 2		5 4 0		5 4 4		6 6 1		7 6 1		8 6 0
24	4 2 2		4 4 3	58	7 3 0				6 5 5		

1.4.2.1. *Symmorphic space groups*

The 73 space groups known as 'symmorphic' are in one-to-one correspondence with the arithmetic crystal classes, and their standard 'short' symbols (Bertaut, 1995) are obtained by interchanging the order of the geometric crystal class and the Bravais cell in the symbol for the arithmetic space group. In fact, conventional crystallographic symbolism did not distinguish between arithmetic crystal classes and symmorphic space groups until recently (de Wolff *et al.*, 1985); the symbol of the symmorphic group was used also for the arithmetic class.

This relationship between the symbols, and the equivalent rule-of-thumb *symmorphic space groups are those whose standard (short) symbols do not contain glide planes or screw axes*, reveal nothing fundamental about the nature of symmorphism; they are simply a consequence of the conventions governing the construction of symbols in *International Tables for Crystallography*.*

Although the *standard* symbols of the symmorphic space groups do not contain screw axes or glide planes, this is a result of the manner in which the space-group symbols have been devised. Most symmorphic space groups do in fact contain screw axes and/or glide planes. This is immediately obvious for the symmorphic space groups based on centred cells; $C2$ contains equal numbers of diad rotation axes and diad screw axes, and Cm contains equal numbers of reflection planes and glide planes. This is recognized in the 'extended' space-group symbols (Bertaut, 1995), but these are clumsy and not commonly used; those for $C2$ and Cm are $C1^{2}_{2_1}1$ and $C1^{m}_{a}1$, respectively. In the more symmetric crystal systems, even symmorphic space groups with primitive cells contain screw axes and/or glide planes; $P422$ ($P42^{2}_{2_1}$) contains many diad screw axes and $P4/mmm$ ($P4/m2/m^{2/m}_{2_1/g}$) contains both screw axes and glide planes.

* Three examples of informative definitions are:

1. The space group corresponding to the zero solution of the Frobenius congruences is called a symmorphic space group (Engel, 1986, p. 155).

2. A space group F is called *symmorphic* if one of its finite subgroups (and therefore an infinity of them) is of an order equal to the order of the point group R_r (Opechowski, 1986, p. 255).

3. A space group is called *symmorphic* if the coset representatives W_j can be chosen in such a way that they leave one common point fixed (Wondratschek, 1995, p. 717).

Even in context, these are pretty opaque.

The balance of symmetry elements within the symmorphic space groups is discussed in more detail in Subsection 9.7.1.2.

1.4.3. Effect of dispersion on diffraction symmetry

In the absence of dispersion ('anomalous scattering'), the intensities of the reflections hkl and $\bar{h}\bar{k}\bar{l}$ are equal (Friedel's law), and statements about the symmetry of the weighted reciprocal lattice and quantities derived from it often rest on the tacit or explicit assumption of this law – the condition underlying it being forgotten. In particular, if dispersion is appreciable, the symmetry of the Patterson synthesis and the 'Laue' symmetry are altered.

1.4.3.1. *Symmetry of the Patterson function*

In Volume A of *International Tables*, the symmetry of the Patterson synthesis is derived in two stages. First, any glide planes and screw axes are replaced by mirror planes and the corresponding rotation axes, giving a symmorphic space group (Subsection 1.4.2.1). Second, a centre of symmetry is added. This second step involves the tacit assumption of Friedel's law, and should not be taken if any atomic scattering factors have appreciable imaginary components. In such cases, the symmetry of the Patterson synthesis will not be that of one of the 24 centrosymmetric symmorphic space groups, as given in Volume A, but will be that of the symmorphic space group belonging to the arithmetic crystal class to which the space group of the structure belongs. There are thus 73 possible Patterson symmetries.

An equivalent description of such symmetries, in terms of 73 of the 1651 dichromatic colour groups, has been given by Fischer & Knop (1987); see also Wilson (1993).

1.4.3.2. *'Laue' symmetry*

Similarly, the eleven conventional 'Laue' symmetries [*International Tables for Crystallography* (1995), Volume A, p. 40 and elsewhere] involve the explicit assumption of Friedel's law. If dispersion is appreciable, the 'Laue' symmetry may be that of any of the 32 point groups. The point group, in correct orientation, is obtained by dropping the Bravais-lattice symbol from the symbol of the arithmetic crystal class or of the Patterson symmetry.

References

1.1–1.3

Cahn, R. W. (1954). *Twinned crystals. Adv. Phys.* **3**, 363–445.

Catti, M. & Ferraris, G. (1976). *Twinning by merohedry and X-ray crystal structure determination. Acta Cryst.* A**32**, 163–165.

Donnay, G. & Donnay, J. D. H. (1974). *Classification of triperiodic twins. Can. Mineral.* **12**, 422–425.

Flack, H. D. (1987). *The derivation of twin laws for (pseudo-) merohedry by coset decomposition. Acta Cryst.* A**43**, 564–568.

Grimmer, H. (1984). *The generating function for coincidence site lattices in the cubic system. Acta Cryst.* A**40**, 108–112.

Grimmer, H. (1989*a*). *Systematic determination of coincidence orientations for all hexagonal lattices with axial ratios c/a in a given interval. Acta Cryst.* A**45**, 320–325.

Grimmer, H. (1989*b*). *Coincidence orientations of grains in rhombohedral materials. Acta Cryst.* A**45**, 505–523.

Grimmer, H. & Warrington, D. H. (1985). *Coincidence orientations of grains in hexagonal materials. J. Phys (Paris),* **46**, C4, 231–236.

Hahn, Th. (1981). *Meroedrische Zwillinge, Symmetrie, Domänen, Kristallstrukturbestimmung. Z. Kristallogr.* **156**, 114–115, and private communication.

Hahn, Th. (1984). *Twin domains and twin boundaries. Acta Cryst.* A**40**, C-117.

International Tables for Crystallography (1983). Vol. A. Dordrecht: Reidel.

International Tables for Crystallography (1987). Vol. A, second, revised ed. Dordrecht: Kluwer Academic Publishers.

Klapper, H. (1987). *X-ray topography of twinned crystals. Prog. Cryst. Growth Charact.* **14**, 367–401.

1.1–1.3 (*cont.*)

Klapper, H., Hahn, Th. & Chung, S. J. (1987). *Optical, pyroelectric and X-ray topographic studies of twin domains and twin boundaries in $KLiSO_4$. Acta Cryst*. B**43**, 147–159.

LePage, Y., Donnay, J. D. H. & Donnay, G. (1984). *Printing sets of structure factors for coping with orientation ambiguities and possible twinning by merohedry*. *Acta Cryst*. A**40**, 679–684.

1.4

Bertaut, E. F. (1995). *Synoptic tables of space-group symbols. Group–subgroup relations*. In *International tables for crystallography*, Vol. A, edited by Th. Hahn, pp. 50–68. Dordrecht: Kluwer Academic Publishers.

Brown, H., Bülow, R., Neubüser, J., Wondratschek, H. & Zassenhaus, H. (1978). *Crystallographic groups of four-dimensional space*. New York: Wiley.

Engel, P. (1986). *Geometric crystallography*. Dordrecht: Reidel. (Present distributor Kluwer Academic Publishers, Dordrecht.)

Fischer, K. F. & Knop, W. E. (1987). *Space groups for imaginary Patterson and for difference Patterson functions in the lambda technique*. *Z. Kristallogr*. **180**, 237-242.

Hahn, Th. (1995). Editor. *International tables for crystallography*, Vol. A. *Space-group symmetry*, fourth, revised, ed. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (1995). Vol. A. *Space-group symmetry,* fourth, revised ed., edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.

Opechowski, W. (1986). *Crystallographic and metacrystallographic groups*. Amsterdam: North Holland.

Wilson, A. J. C. (1993). *Laue and Patterson symmetry in the complex case*. *Z. Kristallogr*. **208**, 199–206.

Wolff, P. M. de, Belov, N. V., Bertaut, E. F., Buerger, M. J., Donnay, J. D. H., Fischer, W., Hahn, Th., Koptsik, V. A., Mackay, A. L., Wondratschek, H., Wilson, A. J. C. & Abrahams, S. C. (1985). *Nomenclature for crystal families, Bravais-lattice types and arithmetic classes*. *Acta Cryst*. A**41**, 278–280.

Wondratschek, H. (1995). *Introduction to space-group symmetry*. *International tables for crystallography*, Vol. A, edited by Th. Hahn, pp. 712–735. Dordrecht: Kluwer Academic Publishers.

references