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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:	

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

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

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

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

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

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

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

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

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

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:	

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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

with

references