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 $s \le 100$, all corresponding pairs $h, k$ are listed in Table 1.2.4.1.

Table 1.2.4.1. *Assignment of integers $s \le 100$ 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:

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

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

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

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

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

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

with





references