International Tables for Crystallography (2006). Vol. C, Section 1.2.5, pp. 7–9.

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.

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

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

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

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

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

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

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

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.

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

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

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

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:

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

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

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

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

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

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

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.

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

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

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

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		

references