International Tables for Crystallography (2006). Vol. C, Section 1.2.5.2, pp. 8–9.

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
1	1	0
3	1	1
4	2	0
7	2	1
9	3	0
12	2	2
13	3	1
16	4	0
19	3	2
21	4	1
25	5	0
27	3	3
28	4	2
31	5	1
36	6	0
37	4	3
39	5	2
43	6	1
48	4	4
49	7	0
	5	3
52	6	2
57	7	1
61	5	4
63	6	3
64	8	0
67	7	2
73	8	1
75	5	5
76	6	4
79	7	3
81	9	0
84	8	2
91	9	1
	6	5
93	7	4
97	8	3
100	10	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
1	0	1	0	0
2	−1	−1	1	0
	1	1	1	0
3	−1	−1	1	1
	3	1	1	1
4	0	2	0	0
5	−2	−2	1	0
	2	2	1	0
6	−3	−2	1	1
	−1	2	−1	1
	5	2	1	1
8	−4	−2	2	0
	4	2	2	0
9	−4	−2	2	1
	0	3	0	0
		2	2	−1
	8	2	2	1
10	−3	−3	1	0
	3	3	1	0
11	−5	−3	1	1
	−1	3	−1	1
	7	3	1	1
12	−4	−2	2	2
	12	2	2	2
13	−6	−3	2	0
	6	3	2	0
14	−7	−3	2	1
	−5	3	−2	1
	1	3	2	−1
	11	3	2	1
16	0	4	0	0
17	−8	−3	2	2
	−4	−4	1	0
		3	−2	2
	4	4	1	0
	16	3	2	2
18	−9	−3	3	0
	−7	−4	1	1
	−1	4	−1	1
	9	4	1	1
		3	3	0
19	−9	−3	3	1
	3	3	3	−1
	15	3	3	1
20	−8	−4	2	0
	8	4	2	0
21	−10	−4	2	1
	−6	4	−2	1
	2	4	2	−1
	14	4	2	1
22	−9	−3	3	2
	−3	3	3	−2
	21	3	3	2
24	−12	−4	2	2
	−4	4	−2	2
	20	4	2	2
25	−12	−4	3	0
	0	5	0	0
	12	4	3	0
26	−13	−4	3	1
	−11	4	−3	1
	−5	−5	1	0
	5	5	1	0
		4	3	−1
	19	4	3	1
27	−9	−5	1	1
		−3	3	3
	−1	5	−1	1
	11	5	1	1
	27	3	3	3
29	−14	−4	3	2
	−10	−5	2	0
		4	−3	2
	−2	4	3	−2
	10	5	2	0
	26	4	3	2
30	−13	−5	2	1
	−7	5	−2	1
	3	5	2	−1
	17	5	2	1
32	−16	−4	4	0
	16	4	4	0
33	−16	−5	2	2
		−4	4	1
	−4	5	−2	2
	8	4	4	−1
	24	5	2	2
		4	4	1
34	−15	−5	3	0
		−4	3	3
	−9	4	−3	3
	15	5	3	0
	33	4	3	3
35	−17	−5	3	1
	−13	5	−3	1
	7	5	3	−1
	23	5	3	1
36	−16	−4	4	2
	0	6	0	0
		4	4	−2
	32	4	4	2
37	−6	−6	1	0
	6	6	1	0
38	−19	−5	3	2
	−11	−6	1	1
		5	−3	2
	−1	6	−1	1
		5	3	−2
	13	6	1	1
	31	5	3	2
40	−12	−6	2	0
	12	6	2	0
41	−20	−5	4	0
	−16	−6	2	1
		−4	4	3
	−8	6	−2	1
		4	4	−3
	4	6	2	−1
	20	6	2	1
		5	4	0
	40	4	4	3
42	−21	−5	4	1
	−19	5	−4	1
	11	5	4	−1
	29	5	4	1
43	−21	−5	3	3
	−9	5	−3	3
	39	5	3	3
44	−20	−6	2	2
	−4	6	−2	2
	28	6	2	2
45	−22	−5	4	2
	−18	−6	3	0
		5	−4	2
	2	5	4	−2
	18	6	3	0
	38	5	4	2
46	−21	−6	3	1
	−15	6	−3	1
	9	6	3	−1
	27	6	3	1
48	−16	−4	4	4
	48	4	4	4
49	−24	−6	3	2
	−12	6	−3	2
	0	7	0	0
		6	3	−2
	36	6	3	2
50	−25	−5	5	0
	−23	−5	4	3
	−17	5	−4	3
	−7	−7	1	0
		5	4	−3
	7	7	1	0
	25	5	5	0
	47	5	4	3

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

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

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

with

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

For each value of $s_1 \le 50$, 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 $s \le 100$, 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 $s \le 100$ 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