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

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

Simplified formulae:

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

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

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

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

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

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

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