

1. CRYSTAL GEOMETRY AND SYMMETRY

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	53	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.

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

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

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

1.2.5.2. Description referred to rhombohedral axes

Metrical conditions:  $a = b = c; \alpha = \beta = \gamma$   
 Bravais lattice type:  $\bar{h}R$   
 Symmetry of lattice points:  $\bar{3}m$   
 Simplified formulae:

$$V = (\mathbf{abc}) = \begin{vmatrix} a^2 & a^2 \cos \alpha & a^2 \cos \alpha \\ a^2 \cos \alpha & a^2 & a^2 \cos \alpha \\ a^2 \cos \alpha & a^2 \cos \alpha & a^2 \end{vmatrix}^{1/2}$$

$$= a^3 [1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha]^{1/2}$$

$$= 2a^3 \left[ \sin \frac{3}{2} \alpha \sin \frac{3}{2} \alpha \right]^{1/2}, \quad (1.1.1.1f)$$

$$\left. \begin{aligned} \cos \frac{\alpha^*}{2} = \cos \frac{\beta^*}{2} = \cos \frac{\gamma^*}{2} = \frac{1}{2 \cos \alpha / 2}, \\ a^* = b^* = c^* = \frac{1}{a \sin \alpha \sin \alpha^*}, \end{aligned} \right\} \quad (1.1.1.3f)$$

$$V^* = (\mathbf{a}^* \mathbf{b}^* \mathbf{c}^*)$$

$$= \begin{vmatrix} a^{*2} & a^{*2} \cos \alpha^* & a^{*2} \cos \alpha^* \\ a^{*2} \cos \alpha^* & a^{*2} & a^{*2} \cos \alpha^* \\ a^{*2} \cos \alpha^* & a^{*2} \cos \alpha^* & a^{*2} \end{vmatrix}^{1/2}$$

$$= a^{*3} [1 - 3 \cos^2 \alpha^* + 2 \cos^3 \alpha^*]^{1/2}$$

$$= 2a^{*3} \left[ \sin \frac{3}{2} \alpha^* \sin \frac{3}{2} \alpha^* \right]^{1/2}, \quad (1.1.1.4f)$$

Table 1.2.5.2. Assignment 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

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

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