

SG No. 178  $D_6^2$   $P6_122$  [ hexagonal ]

\* plus set:  $+ [0, 0, 0]$

\* Wyckoff site: **6a**, site symmetry:  $.2$ .

Table 1: Wyckoff bond: **6a@6a**

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[x, 0, 0]$	$[1, -8]$
2	$[-2X, -X, Z]$	$[0, x, \frac{1}{3}]$	$[2, -7]$
3	$[X, -X, Z]$	$[-x, -x, \frac{2}{3}]$	$[3, -9]$
4	$[-X, -2X, Z]$	$[-x, 0, \frac{1}{2}]$	$[4, -11]$
5	$[2X, X, Z]$	$[0, -x, \frac{5}{6}]$	$[5, -10]$
6	$[-X, X, Z]$	$[x, x, \frac{1}{6}]$	$[6, -12]$

Table 2: Wyckoff bond: **6b@6a**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	$[1, 8]$
2	$[0, X, 0]$	$[0, x, \frac{1}{3}]$	$[2, 7]$
3	$[-X, -X, 0]$	$[-x, -x, \frac{2}{3}]$	$[3, 9]$
4	$[-X, 0, 0]$	$[-x, 0, \frac{1}{2}]$	$[4, 11]$
5	$[0, -X, 0]$	$[0, -x, \frac{5}{6}]$	$[5, 10]$
6	$[X, X, 0]$	$[x, x, \frac{1}{6}]$	$[6, 12]$

Table 3: Wyckoff bond: **12c@6a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, 0]$	$[1]$
2	$[-Y, X - Y, Z]$	$[0, x, \frac{1}{3}]$	$[2]$
3	$[-X + Y, -X, Z]$	$[-x, -x, \frac{2}{3}]$	$[3]$
4	$[-X, -Y, Z]$	$[-x, 0, \frac{1}{2}]$	$[4]$
5	$[Y, -X + Y, Z]$	$[0, -x, \frac{5}{6}]$	$[5]$
6	$[X - Y, X, Z]$	$[x, x, \frac{1}{6}]$	$[6]$
7	$[Y, X, -Z]$	$[0, x, \frac{1}{3}]$	$[7]$
8	$[X - Y, -Y, -Z]$	$[x, 0, 0]$	$[8]$
9	$[-X, -X + Y, -Z]$	$[-x, -x, \frac{2}{3}]$	$[9]$
10	$[-Y, -X, -Z]$	$[0, -x, \frac{5}{6}]$	$[10]$
11	$[-X + Y, Y, -Z]$	$[-x, 0, \frac{1}{2}]$	$[11]$
12	$[X, X - Y, -Z]$	$[x, x, \frac{1}{6}]$	$[12]$

\* Wyckoff site: **6b**, site symmetry:  $. . 2$

Table 4: Wyckoff bond: **6a@6b**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 2x, \frac{1}{4}]$	$[1, -11]$
2	$[0, X, Z]$	$[-2x, -x, \frac{7}{12}]$	$[2, -10]$
3	$[-X, -X, Z]$	$[x, -x, \frac{11}{12}]$	$[3, -12]$
4	$[-X, 0, Z]$	$[-x, -2x, \frac{3}{4}]$	$[4, -8]$
5	$[0, -X, Z]$	$[2x, x, \frac{1}{12}]$	$[5, -7]$
6	$[X, X, Z]$	$[-x, x, \frac{5}{12}]$	$[6, -9]$

Table 5: Wyckoff bond: **6b@6b**

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[x, 2x, \frac{1}{4}]$	$[1, 11]$
2	$[-2X, -X, 0]$	$[-2x, -x, \frac{7}{12}]$	$[2, 10]$
3	$[X, -X, 0]$	$[x, -x, \frac{11}{12}]$	$[3, 12]$
4	$[-X, -2X, 0]$	$[-x, -2x, \frac{3}{4}]$	$[4, 8]$
5	$[2X, X, 0]$	$[2x, x, \frac{1}{12}]$	$[5, 7]$
6	$[-X, X, 0]$	$[-x, x, \frac{5}{12}]$	$[6, 9]$

Table 6: Wyckoff bond: **12c@6b**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 2x, \frac{1}{4}]$	$[1]$
2	$[-Y, X - Y, Z]$	$[-2x, -x, \frac{7}{12}]$	$[2]$
3	$[-X + Y, -X, Z]$	$[x, -x, \frac{11}{12}]$	$[3]$
4	$[-X, -Y, Z]$	$[-x, -2x, \frac{3}{4}]$	$[4]$
5	$[Y, -X + Y, Z]$	$[2x, x, \frac{1}{12}]$	$[5]$
6	$[X - Y, X, Z]$	$[-x, x, \frac{5}{12}]$	$[6]$
7	$[Y, X, -Z]$	$[2x, x, \frac{1}{12}]$	$[7]$
8	$[X - Y, -Y, -Z]$	$[-x, -2x, \frac{3}{4}]$	$[8]$
9	$[-X, -X + Y, -Z]$	$[-x, x, \frac{5}{12}]$	$[9]$
10	$[-Y, -X, -Z]$	$[-2x, -x, \frac{7}{12}]$	$[10]$
11	$[-X + Y, Y, -Z]$	$[x, 2x, \frac{1}{4}]$	$[11]$
12	$[X, X - Y, -Z]$	$[x, -x, \frac{11}{12}]$	$[12]$

\* Wyckoff site: 12c, site symmetry: 1

Table 7: Wyckoff bond: **12a@12c**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	$[1]$

*continued ...*

Table 7

No.	vector	center	mapping
2	$[-Y, X - Y, Z]$	$[-y, x - y, z + \frac{1}{3}]$	[2]
3	$[-X + Y, -X, Z]$	$[-x + y, -x, z + \frac{2}{3}]$	[3]
4	$[-X, -Y, Z]$	$[-x, -y, z + \frac{1}{2}]$	[4]
5	$[Y, -X + Y, Z]$	$[y, -x + y, z + \frac{5}{6}]$	[5]
6	$[X - Y, X, Z]$	$[x - y, x, z + \frac{1}{6}]$	[6]
7	$[Y, X, -Z]$	$[y, x, \frac{1}{3} - z]$	[7]
8	$[X - Y, -Y, -Z]$	$[x - y, -y, -z]$	[8]
9	$[-X, -X + Y, -Z]$	$[-x, -x + y, \frac{2}{3} - z]$	[9]
10	$[-Y, -X, -Z]$	$[-y, -x, \frac{5}{6} - z]$	[10]
11	$[-X + Y, Y, -Z]$	$[-x + y, y, \frac{1}{2} - z]$	[11]
12	$[X, X - Y, -Z]$	$[x, x - y, \frac{1}{6} - z]$	[12]