

SG No. 184  $C_{6v}^2$   $P6cc$  [ hexagonal ]

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

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

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 6b@2a

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

Table 3: Wyckoff bond: 12c@2a

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

\* Wyckoff site: 4b, site symmetry: 3..

Table 4: Wyckoff bond: 4a@4b

No.	vector	center	mapping
1	[0, 0, Z]	[\frac{1}{3}, \frac{2}{3}, z]	[1,2,3]

*continued ...*

Table 4

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

Table 5: Wyckoff bond: 12b@4b

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

\* Wyckoff site: 6c, site symmetry: 2..

Table 6: Wyckoff bond: 6a@6c

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

Table 7: Wyckoff bond: 6b@6c

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, z]$	[1,4]
2	$[0, 0, Z]$	$[0, \frac{1}{2}, z]$	[2,5]
3	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[3,6]
4	$[0, 0, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[7,10]
5	$[0, 0, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[8,11]

*continued ...*

Table 7

No.	vector	center	mapping
6	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9,12]

Table 8: Wyckoff bond: 12c@6c

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

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

Table 9: Wyckoff bond: 12a@12d

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