

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]