

SG No. 179 D_6^3 $P6_522$ [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	$[-2X, -X, Z]$	$[0, x, \frac{2}{3}]$	[2,-7]
3	$[X, -X, Z]$	$[-x, -x, \frac{1}{3}]$	[3,-9]
4	$[-X, -2X, Z]$	$[-x, 0, \frac{1}{2}]$	[4,-11]
5	$[2X, X, Z]$	$[0, -x, \frac{1}{6}]$	[5,-10]
6	$[-X, X, Z]$	$[x, x, \frac{5}{6}]$	[6,-12]

Table 2: Wyckoff bond: 6b@6a

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

Table 3: Wyckoff bond: 12c@6a

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

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

Table 4: Wyckoff bond: 6a@6b

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

Table 5: Wyckoff bond: 6b@6b

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

Table 6: Wyckoff bond: 12c@6b

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