

SG No. 158 C_{3v}^3 $P3c1$ [trigonal]

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

* Wyckoff site: 2a, site symmetry: 3..

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 6b@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	[-Y, -X, Z]	[0, 0, $z + \frac{1}{2}$]	[4]
5	[-X + Y, Y, Z]	[0, 0, $z + \frac{1}{2}$]	[5]
6	[X, X - Y, Z]	[0, 0, $z + \frac{1}{2}$]	[6]

* Wyckoff site: 2b, site symmetry: 3..

Table 3: Wyckoff bond: 2a@2b

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

Table 4: Wyckoff bond: 6b@2b

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	[-Y, -X, Z]	[\frac{1}{3}, \frac{2}{3}, $z + \frac{1}{2}$]	[4]
5	[-X + Y, Y, Z]	[\frac{1}{3}, \frac{2}{3}, $z + \frac{1}{2}$]	[5]
6	[X, X - Y, Z]	[\frac{1}{3}, \frac{2}{3}, $z + \frac{1}{2}$]	[6]

* Wyckoff site: 2c, site symmetry: 3..

Table 5: Wyckoff bond: 2a@2c

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

Table 6: Wyckoff bond: 6b@2c

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

* Wyckoff site: 6d, site symmetry: 1

Table 7: Wyckoff bond: 6a@6d

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	[-Y, -X, Z]	[-y, -x, z + $\frac{1}{2}$]	[4]
5	[-X + Y, Y, Z]	[-x + y, y, z + $\frac{1}{2}$]	[5]
6	[X, X - Y, Z]	[x, x - y, z + $\frac{1}{2}$]	[6]