

SG No. 159  $C_{3v}^4$   $P31c$  [ 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{2}{3}, \frac{1}{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{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: 6c, site symmetry: 1

Table 5: Wyckoff bond: 6a@6c

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]