

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