

SG No. 152  $D_3^4$   $P3_121$  [ trigonal ]

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

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

Table 1: Wyckoff bond: 3a@3a

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

Table 2: Wyckoff bond: 3b@3a

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, \frac{1}{3}]$	[1, 5]
2	$[0, X, 0]$	$[0, x, \frac{2}{3}]$	[2, 4]
3	$[-X, -X, 0]$	$[-x, -x, 0]$	[3, 6]

Table 3: Wyckoff bond: 6c@3a

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

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

Table 4: Wyckoff bond: 3a@3b

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

Table 5: Wyckoff bond: **3b@3b**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, \frac{5}{6}]$	[1, 5]
2	$[0, X, 0]$	$[0, x, \frac{1}{6}]$	[2, 4]
3	$[-X, -X, 0]$	$[-x, -x, \frac{1}{2}]$	[3, 6]

Table 6: Wyckoff bond: **6c@3b**

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

\* Wyckoff site: **6c**, site symmetry: **1**

Table 7: Wyckoff bond: **6a@6c**

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