

SG No. 151 D_3^3 $P3_112$ [trigonal]

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

* Wyckoff site: **3a**, site symmetry: $\bar{3}..2$

Table 1: Wyckoff bond: **3a@3a**

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

Table 2: Wyckoff bond: **3b@3a**

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

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

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

* Wyckoff site: **3b**, site symmetry: $\bar{3}..2$

Table 4: Wyckoff bond: **3a@3b**

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

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

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

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

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

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