

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