

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

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

* Wyckoff site: 3a, site symmetry: . . 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: . . 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]