

SG No. 156 C_{3v}^1 $P3m1$ [trigonal]

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

* Wyckoff site: 1a, site symmetry: 3m.

Table 1: Wyckoff bond: 1a@1a

No.	vector	center	mapping
1	[0, 0, Z]	[0, 0, z]	[1,2,3,4,5,6]

Table 2: Wyckoff bond: 3b@1a

No.	vector	center	mapping
1	[X, -X, Z]	[0, 0, z]	[1,4]
2	[X, 2X, Z]	[0, 0, z]	[2,6]
3	[-2X, -X, Z]	[0, 0, z]	[3,5]

Table 3: Wyckoff bond: 3c@1a

No.	vector	center	mapping
1	[X, 0, 0]	[0, 0, z]	[1,-5]
2	[0, X, 0]	[0, 0, z]	[2,-4]
3	[-X, -X, 0]	[0, 0, z]	[3,-6]

Table 4: Wyckoff bond: 6d@1a

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]	[4]
5	[-X + Y, Y, Z]	[0, 0, z]	[5]
6	[X, X - Y, Z]	[0, 0, z]	[6]

* Wyckoff site: 1b, site symmetry: 3m.

Table 5: Wyckoff bond: 1a@1b

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

Table 6: Wyckoff bond: 3b@1b

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

Table 7: Wyckoff bond: 3c@1b

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

Table 8: Wyckoff bond: 6d@1b

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

* Wyckoff site: 1c, site symmetry: 3m.

Table 9: Wyckoff bond: 1a@1c

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

Table 10: Wyckoff bond: 3b@1c

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

Table 11: Wyckoff bond: 3c@1c

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

Table 12: Wyckoff bond: 6d@1c

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

* Wyckoff site: 3d, site symmetry: .m.

Table 13: Wyckoff bond: 3a@3d

No.	vector	center	mapping
1	[X, -X, Z]	[x, -x, z]	[1, 4]
2	[X, 2X, Z]	[x, 2x, z]	[2, 6]
3	[-2X, -X, Z]	[-2x, -x, z]	[3, 5]

Table 14: Wyckoff bond: 3b@3d

No.	vector	center	mapping
1	[X, X, 0]	[x, -x, z]	[1, -4]
2	[-X, 0, 0]	[x, 2x, z]	[2, -6]
3	[0, -X, 0]	[-2x, -x, z]	[3, -5]

Table 15: Wyckoff bond: 6c@3d

No.	vector	center	mapping
1	[X, Y, Z]	[x, -x, z]	[1]
2	[-Y, X - Y, Z]	[x, 2x, z]	[2]
3	[-X + Y, -X, Z]	[-2x, -x, z]	[3]
4	[-Y, -X, Z]	[x, -x, z]	[4]

continued ...

Table 15

No.	vector	center	mapping
5	$[-X + Y, Y, Z]$	$[-2x, -x, z]$	[5]
6	$[X, X - Y, Z]$	$[x, 2x, z]$	[6]

* Wyckoff site: **6e**, site symmetry: 1

Table 16: Wyckoff bond: **6a@6e**

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	$[-Y, -X, Z]$	$[-y, -x, z]$	[4]
5	$[-X + Y, Y, Z]$	$[-x + y, y, z]$	[5]
6	$[X, X - Y, Z]$	$[x, x - y, z]$	[6]