

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]