

SG No. 150 D_3^2 $P321$ [trigonal]

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

* Wyckoff site: **1a**, site symmetry: **32**.

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

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

Table 2: Wyckoff bond: **3b@1a**

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

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

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

Table 4: Wyckoff bond: **6d@1a**

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

* Wyckoff site: **1b**, site symmetry: **32**.

Table 5: Wyckoff bond: **1a@1b**

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

Table 6: Wyckoff bond: **3b@1b**

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

Table 7: Wyckoff bond: **3c@1b**

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

Table 8: Wyckoff bond: **6d@1b**

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

* Wyckoff site: **2c**, site symmetry: **3..**

Table 9: Wyckoff bond: **2a@2c**

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

Table 10: Wyckoff bond: **6b@2c**

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	$[X - Y, -Y, -Z]$	$[0, 0, -z]$	$[5]$

continued ...

Table 10

No.	vector	center	mapping
6	$[-X, -X + Y, -Z]$	$[0, 0, -z]$	[6]

* Wyckoff site: 2d, site symmetry: $3..$

Table 11: Wyckoff bond: 2a@2d

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

Table 12: Wyckoff bond: 6b@2d

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	$[Y, X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, -z]$	[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: 3e, site symmetry: $.2.$

Table 13: Wyckoff bond: 3a@3e

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

Table 14: Wyckoff bond: 3b@3e

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

Table 15: Wyckoff bond: **6c@3e**

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

* Wyckoff site: **3f**, site symmetry: $.2$.

Table 16: Wyckoff bond: **3a@3f**

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

Table 17: Wyckoff bond: **3b@3f**

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

Table 18: Wyckoff bond: **6c@3f**

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

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

Table 19: Wyckoff bond: $6a@6g$

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]