

SG No. 183 $C_{6v}^1 P6mm$ [hexagonal]

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

* Wyckoff site: 1a, site symmetry: 6mm

Table 1: Wyckoff bond: 1a@1a

No.	vector	center	mapping
1	[0, 0, Z]	[0, 0, z]	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]

Table 2: Wyckoff bond: 3b@1a

No.	vector	center	mapping
1	[X, 2X, 0]	[0, 0, z]	[1, -4, 8, -11]
2	[-2X, -X, 0]	[0, 0, z]	[2, -5, 7, -10]
3	[X, -X, 0]	[0, 0, z]	[3, -6, 9, -12]

Table 3: Wyckoff bond: 3c@1a

No.	vector	center	mapping
1	[X, 0, 0]	[0, 0, z]	[1, -4, -8, 11]
2	[0, X, 0]	[0, 0, z]	[2, -5, -7, 10]
3	[-X, -X, 0]	[0, 0, z]	[3, -6, -9, 12]

Table 4: Wyckoff bond: 6d@1a

No.	vector	center	mapping
1	[X, Y, 0]	[0, 0, z]	[1, -4]
2	[-Y, X - Y, 0]	[0, 0, z]	[2, -5]
3	[-X + Y, -X, 0]	[0, 0, z]	[3, -6]
4	[-Y, -X, 0]	[0, 0, z]	[7, -10]
5	[-X + Y, Y, 0]	[0, 0, z]	[8, -11]
6	[X, X - Y, 0]	[0, 0, z]	[9, -12]

Table 5: Wyckoff bond: 6e@1a

No.	vector	center	mapping
1	[X, 2X, Z]	[0, 0, z]	[1, 8]
2	[-2X, -X, Z]	[0, 0, z]	[2, 7]
3	[X, -X, Z]	[0, 0, z]	[3, 9]

continued ...

Table 5

No.	vector	center	mapping
4	$[-X, -2X, Z]$	$[0, 0, z]$	$[4, 11]$
5	$[2X, X, Z]$	$[0, 0, z]$	$[5, 10]$
6	$[-X, X, Z]$	$[0, 0, z]$	$[6, 12]$

Table 6: Wyckoff bond: **6f@1a**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, z]$	$[1, 11]$
2	$[0, X, Z]$	$[0, 0, z]$	$[2, 10]$
3	$[-X, -X, Z]$	$[0, 0, z]$	$[3, 12]$
4	$[-X, 0, Z]$	$[0, 0, z]$	$[4, 8]$
5	$[0, -X, Z]$	$[0, 0, z]$	$[5, 7]$
6	$[X, X, Z]$	$[0, 0, z]$	$[6, 9]$

Table 7: Wyckoff bond: **12g@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	$[-X, -Y, Z]$	$[0, 0, z]$	$[4]$
5	$[Y, -X + Y, Z]$	$[0, 0, z]$	$[5]$
6	$[X - Y, X, Z]$	$[0, 0, z]$	$[6]$
7	$[-Y, -X, Z]$	$[0, 0, z]$	$[7]$
8	$[-X + Y, Y, Z]$	$[0, 0, z]$	$[8]$
9	$[X, X - Y, Z]$	$[0, 0, z]$	$[9]$
10	$[Y, X, Z]$	$[0, 0, z]$	$[10]$
11	$[X - Y, -Y, Z]$	$[0, 0, z]$	$[11]$
12	$[-X, -X + Y, Z]$	$[0, 0, z]$	$[12]$

* Wyckoff site: **2b**, site symmetry: **3m**.

Table 8: Wyckoff bond: **2a@2b**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3, 7, 8, 9]$
2	$[0, 0, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	$[4, 5, 6, 10, 11, 12]$

Table 9: Wyckoff bond: 6b@2b

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[1,8]
2	$[-2X, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[2,7]
3	$[X, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[3,9]
4	$[-X, -2X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[4,11]
5	$[2X, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[5,10]
6	$[-X, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[6,12]

Table 10: Wyckoff bond: 6c@2b

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[1,-8]
2	$[0, X, 0]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[2,-7]
3	$[-X, -X, 0]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[3,-9]
4	$[-X, 0, 0]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[4,-11]
5	$[0, -X, 0]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[5,-10]
6	$[X, X, 0]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[6,-12]

Table 11: Wyckoff bond: 12d@2b

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	$[-X, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[4]
5	$[Y, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[5]
6	$[X - Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[6]
7	$[-Y, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[7]
8	$[-X + Y, Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[8]
9	$[X, X - Y, Z]$	$[\frac{1}{3}, \frac{2}{3}, z]$	[9]
10	$[Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[10]
11	$[X - Y, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[11]
12	$[-X, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z]$	[12]

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

Table 12: Wyckoff bond: 3a@3c

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[\frac{1}{2}, 0, z]$	[1,-4,8,-11]

continued ...

Table 12

No.	vector	center	mapping
2	$[-2X, -X, 0]$	$[0, \frac{1}{2}, z]$	$[2, -5, 7, -10]$
3	$[X, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[3, -6, 9, -12]$

Table 13: Wyckoff bond: 3b@3c

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, 0, z]$	$[1, -4, -8, 11]$
2	$[0, X, 0]$	$[0, \frac{1}{2}, z]$	$[2, -5, -7, 10]$
3	$[-X, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[3, -6, -9, 12]$

Table 14: Wyckoff bond: 3c@3c

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, z]$	$[1, 4, 8, 11]$
2	$[0, 0, Z]$	$[0, \frac{1}{2}, z]$	$[2, 5, 7, 10]$
3	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[3, 6, 9, 12]$

Table 15: Wyckoff bond: 6d@3c

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, z]$	$[1, -4]$
2	$[-Y, X - Y, 0]$	$[0, \frac{1}{2}, z]$	$[2, -5]$
3	$[-X + Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[3, -6]$
4	$[-Y, -X, 0]$	$[0, \frac{1}{2}, z]$	$[7, -10]$
5	$[-X + Y, Y, 0]$	$[\frac{1}{2}, 0, z]$	$[8, -11]$
6	$[X, X - Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[9, -12]$

Table 16: Wyckoff bond: 6e@3c

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[\frac{1}{2}, 0, z]$	$[1, 8]$
2	$[-2X, -X, Z]$	$[0, \frac{1}{2}, z]$	$[2, 7]$
3	$[X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[3, 9]$
4	$[-X, -2X, Z]$	$[\frac{1}{2}, 0, z]$	$[4, 11]$
5	$[2X, X, Z]$	$[0, \frac{1}{2}, z]$	$[5, 10]$
6	$[-X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[6, 12]$

Table 17: Wyckoff bond: **6f@3c**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, 0, z]$	[1,11]
2	$[0, X, Z]$	$[0, \frac{1}{2}, z]$	[2,10]
3	$[-X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[3,12]
4	$[-X, 0, Z]$	$[\frac{1}{2}, 0, z]$	[4,8]
5	$[0, -X, Z]$	$[0, \frac{1}{2}, z]$	[5,7]
6	$[X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[6,9]

Table 18: Wyckoff bond: **12g@3c**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, z]$	[1]
2	$[-Y, X - Y, Z]$	$[0, \frac{1}{2}, z]$	[2]
3	$[-X + Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[3]
4	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, z]$	[4]
5	$[Y, -X + Y, Z]$	$[0, \frac{1}{2}, z]$	[5]
6	$[X - Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[6]
7	$[-Y, -X, Z]$	$[0, \frac{1}{2}, z]$	[7]
8	$[-X + Y, Y, Z]$	$[\frac{1}{2}, 0, z]$	[8]
9	$[X, X - Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[9]
10	$[Y, X, Z]$	$[0, \frac{1}{2}, z]$	[10]
11	$[X - Y, -Y, Z]$	$[\frac{1}{2}, 0, z]$	[11]
12	$[-X, -X + Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	[12]

* Wyckoff site: **6d**, site symmetry: $\dots m$

Table 19: Wyckoff bond: **6a@6d**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	[1,11]
2	$[0, X, Z]$	$[0, x, z]$	[2,10]
3	$[-X, -X, Z]$	$[-x, -x, z]$	[3,12]
4	$[-X, 0, Z]$	$[-x, 0, z]$	[4,8]
5	$[0, -X, Z]$	$[0, -x, z]$	[5,7]
6	$[X, X, Z]$	$[x, x, z]$	[6,9]

Table 20: Wyckoff bond: **6b@6d**

No.	vector	center	mapping
1	$[X, 2X, 0]$	$[x, 0, z]$	[1,-11]

continued ...

Table 20

No.	vector	center	mapping
2	$[-2X, -X, 0]$	$[0, x, z]$	$[2, -10]$
3	$[X, -X, 0]$	$[-x, -x, z]$	$[3, -12]$
4	$[-X, -2X, 0]$	$[-x, 0, z]$	$[4, -8]$
5	$[2X, X, 0]$	$[0, -x, z]$	$[5, -7]$
6	$[-X, X, 0]$	$[x, x, z]$	$[6, -9]$

Table 21: Wyckoff bond: $12c@6d$

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, z]$	$[1]$
2	$[-Y, X - Y, Z]$	$[0, x, z]$	$[2]$
3	$[-X + Y, -X, Z]$	$[-x, -x, z]$	$[3]$
4	$[-X, -Y, Z]$	$[-x, 0, z]$	$[4]$
5	$[Y, -X + Y, Z]$	$[0, -x, z]$	$[5]$
6	$[X - Y, X, Z]$	$[x, x, z]$	$[6]$
7	$[-Y, -X, Z]$	$[0, -x, z]$	$[7]$
8	$[-X + Y, Y, Z]$	$[-x, 0, z]$	$[8]$
9	$[X, X - Y, Z]$	$[x, x, z]$	$[9]$
10	$[Y, X, Z]$	$[0, x, z]$	$[10]$
11	$[X - Y, -Y, Z]$	$[x, 0, z]$	$[11]$
12	$[-X, -X + Y, Z]$	$[-x, -x, z]$	$[12]$

* Wyckoff site: $6e$, site symmetry: $.m$.

Table 22: Wyckoff bond: $6a@6e$

No.	vector	center	mapping
1	$[X, -X, Z]$	$[x, -x, z]$	$[1, 7]$
2	$[X, 2X, Z]$	$[x, 2x, z]$	$[2, 9]$
3	$[-2X, -X, Z]$	$[-2x, -x, z]$	$[3, 8]$
4	$[-X, X, Z]$	$[-x, x, z]$	$[4, 10]$
5	$[-X, -2X, Z]$	$[-x, -2x, z]$	$[5, 12]$
6	$[2X, X, Z]$	$[2x, x, z]$	$[6, 11]$

Table 23: Wyckoff bond: $6b@6e$

No.	vector	center	mapping
1	$[X, X, 0]$	$[x, -x, z]$	$[1, -7]$
2	$[-X, 0, 0]$	$[x, 2x, z]$	$[2, -9]$
3	$[0, -X, 0]$	$[-2x, -x, z]$	$[3, -8]$

continued ...

Table 23

No.	vector	center	mapping
4	$[-X, -X, 0]$	$[-x, x, z]$	[4,-10]
5	$[X, 0, 0]$	$[-x, -2x, z]$	[5,-12]
6	$[0, X, 0]$	$[2x, x, z]$	[6,-11]

Table 24: Wyckoff bond: 12c@6e

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	$[-X, -Y, Z]$	$[-x, x, z]$	[4]
5	$[Y, -X + Y, Z]$	$[-x, -2x, z]$	[5]
6	$[X - Y, X, Z]$	$[2x, x, z]$	[6]
7	$[-Y, -X, Z]$	$[x, -x, z]$	[7]
8	$[-X + Y, Y, Z]$	$[-2x, -x, z]$	[8]
9	$[X, X - Y, Z]$	$[x, 2x, z]$	[9]
10	$[Y, X, Z]$	$[-x, x, z]$	[10]
11	$[X - Y, -Y, Z]$	$[2x, x, z]$	[11]
12	$[-X, -X + Y, Z]$	$[-x, -2x, z]$	[12]

* Wyckoff site: 12f, site symmetry: 1

Table 25: Wyckoff bond: 12a@12f

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	$[-X, -Y, Z]$	$[-x, -y, z]$	[4]
5	$[Y, -X + Y, Z]$	$[y, -x + y, z]$	[5]
6	$[X - Y, X, Z]$	$[x - y, x, z]$	[6]
7	$[-Y, -X, Z]$	$[-y, -x, z]$	[7]
8	$[-X + Y, Y, Z]$	$[-x + y, y, z]$	[8]
9	$[X, X - Y, Z]$	$[x, x - y, z]$	[9]
10	$[Y, X, Z]$	$[y, x, z]$	[10]
11	$[X - Y, -Y, Z]$	$[x - y, -y, z]$	[11]
12	$[-X, -X + Y, Z]$	$[-x, -x + y, z]$	[12]