

PG No. 26 D_{3h} $\bar{6}m2$ (-6m2 setting) [hexagonal]

* Wyckoff site: 2a, site symmetry: $3m$.

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 6b@2a

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[0, 0, z]$	$[1, 8]$
2	$[-2X, -X, Z]$	$[0, 0, z]$	$[2, 7]$
3	$[X, -X, Z]$	$[0, 0, z]$	$[3, 9]$
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 3: Wyckoff bond: 6c@2a

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

Table 4: Wyckoff bond: 12d@2a

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	$[-Y, -X, -Z]$	$[0, 0, -z]$	$[10]$

continued ...

Table 4

No.	vector	center	mapping
11	$[-X + Y, Y, -Z]$	$[0, 0, -z]$	[11]
12	$[X, X - Y, -Z]$	$[0, 0, -z]$	[12]

* Wyckoff site: 3b, site symmetry: mm2

Table 5: Wyckoff bond: 3a@3b

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

Table 6: Wyckoff bond: 3b@3b

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

Table 7: Wyckoff bond: 3c@3b

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

Table 8: Wyckoff bond: 6d@3b

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

Table 9: Wyckoff bond: **6e@3b**

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

Table 10: Wyckoff bond: **6f@3b**

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

Table 11: Wyckoff bond: **12g@3b**

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

* Wyckoff site: **6c**, site symmetry: $\cdot m$.

Table 12: Wyckoff bond: **6a@6c**

No.	vector	center	mapping
1	$[X, -X, Z]$	$[x, -x, z]$	$[1, 7]$

continued ...

Table 12

No.	vector	center	mapping
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 13: Wyckoff bond: 6b@6c

No.	vector	center	mapping
1	$[X, X, 0]$	$[x, -x, z]$	$[1, -7]$
2	$[-X, 0, 0]$	$[x, 2x, z]$	$[2, -9]$
3	$[0, -X, 0]$	$[-2x, -x, z]$	$[3, -8]$
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 14: Wyckoff bond: 12c@6c

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: 6d, site symmetry: $m..$

Table 15: Wyckoff bond: 6a@6d

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

continued ...

Table 15

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

Table 16: Wyckoff bond: 6b@6d

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

Table 17: Wyckoff bond: 12c@6d

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

* Wyckoff site: 12e, site symmetry: 1

Table 18: Wyckoff bond: 12a@12e

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]

continued ...

Table 18

No.	vector	center	mapping
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]