

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: .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]