

PG No. 25 C_{6v} $6mm$ [hexagonal]

* 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]
4	[-X, -2X, Z]	[0, 0, z]	[4,11]

continued ...

Table 5

No.	vector	center	mapping
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: 6b, site symmetry: ...m

Table 8: Wyckoff bond: 6a@6b

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 9: Wyckoff bond: 6b@6b

No.	vector	center	mapping
1	[$X, 2X, 0$]	[$x, 0, z$]	[1,-11]
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 10: Wyckoff bond: 12c@6b

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: 6c, site symmetry: .m.

Table 11: Wyckoff bond: 6a@6c

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 12: 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 13: 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: 12d, site symmetry: 1

Table 14: Wyckoff bond: 12a@12d

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]