

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:  $\dots m$

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	$[-X, -X + Y, Z]$	$[-x, -x + y, z]$	$[12]$