

PG No. 24 D_6 622 [hexagonal]

* Wyckoff site: 2a, site symmetry: $6..$

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 6b@2a

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 3: Wyckoff bond: 12c@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	$[-Y, -X, -Z]$	$[0, 0, -z]$	$[10]$
11	$[-X + Y, Y, -Z]$	$[0, 0, -z]$	$[11]$
12	$[X, X - Y, -Z]$	$[0, 0, -z]$	$[12]$

* Wyckoff site: 6b, site symmetry: $.2.$

Table 4: Wyckoff bond: 6a@6b

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

continued ...

Table 4

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

Table 5: Wyckoff bond: **6b@6b**

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

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

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

* Wyckoff site: **6c**, site symmetry: $\cdot \cdot 2$

Table 7: Wyckoff bond: **6a@6c**

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	$[-X, -X, Z]$	$[-x, x, 0]$	$[4, -7]$

continued ...

Table 7

No.	vector	center	mapping
5	$[X, 0, Z]$	$[-x, -2x, 0]$	$[5, -9]$
6	$[0, X, Z]$	$[2x, x, 0]$	$[6, -8]$

Table 8: Wyckoff bond: **6b@6c**

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

Table 9: Wyckoff bond: **12c@6c**

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: **12d**, site symmetry: **1**

Table 10: 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	$[X - Y, X, Z]$	$[x - y, x, z]$	$[6]$

continued ...

Table 10

No.	vector	center	mapping
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]