

PG No. 23  $C_{6h}$   $6/m$  [ 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	$[-X, -Y, 0]$	$[0, 0, -z]$	$[7, -10]$
5	$[Y, -X + Y, 0]$	$[0, 0, -z]$	$[8, -11]$
6	$[X - Y, X, 0]$	$[0, 0, -z]$	$[9, -12]$

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	$[-X, -Y, -Z]$	$[0, 0, -z]$	$[7]$
8	$[Y, -X + Y, -Z]$	$[0, 0, -z]$	$[8]$
9	$[X - Y, X, -Z]$	$[0, 0, -z]$	$[9]$
10	$[X, Y, -Z]$	$[0, 0, -z]$	$[10]$
11	$[-Y, X - Y, -Z]$	$[0, 0, -z]$	$[11]$
12	$[-X + Y, -X, -Z]$	$[0, 0, -z]$	$[12]$

\* Wyckoff site: 6b, site symmetry:  $m..$

Table 4: Wyckoff bond: 6a@6b

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, y, 0]$	$[1, 10]$
2	$[-Y, X - Y, 0]$	$[-y, x - y, 0]$	$[2, 11]$

*continued ...*

Table 4

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

Table 5: Wyckoff bond: 6b@6b

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

Table 6: Wyckoff bond: 12c@6b

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	$[-X, -Y, -Z]$	$[-x, -y, 0]$	[7]
8	$[Y, -X + Y, -Z]$	$[y, -x + y, 0]$	[8]
9	$[X - Y, X, -Z]$	$[x - y, x, 0]$	[9]
10	$[X, Y, -Z]$	$[x, y, 0]$	[10]
11	$[-Y, X - Y, -Z]$	$[-y, x - y, 0]$	[11]
12	$[-X + Y, -X, -Z]$	$[-x + y, -x, 0]$	[12]

\* Wyckoff site: 12c, site symmetry: 1

Table 7: Wyckoff bond: 12a@12c

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]

*continued ...*

Table 7

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