

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]