

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: ..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]