SG No. 186 C_{6v}^4 $P6_3mc$ [hexagonal]

* plus set: $+[0,\ 0,\ 0]$
* Wyckoff site: `2a`, site symmetry: `3m.`

Table 1: Wyckoff bond: `2a@2a`

No.	vector	center	mapping
1	$[0,\ 0,\ Z]$	$[0,\ 0,\ z]$	`[1,2,3,7,8,9]`
2	$[0,\ 0,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[4,5,6,10,11,12]`

Table 2: Wyckoff bond: `6b@2a`

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	$[-X,\ -2X,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[4,11]`
5	$[2X,\ X,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[5,10]`
6	$[-X,\ X,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[6,12]`

Table 3: Wyckoff bond: `6c@2a`

No.	vector	center	mapping
1	$[X,\ 0,\ 0]$	$[0,\ 0,\ z]$	`[1,-8]`
2	$[0,\ X,\ 0]$	$[0,\ 0,\ z]$	`[2,-7]`
3	$[-X,\ -X,\ 0]$	$[0,\ 0,\ z]$	`[3,-9]`
4	$[-X,\ 0,\ 0]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[4,-11]`
5	$[0,\ -X,\ 0]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[5,-10]`
6	$[X,\ X,\ 0]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[6,-12]`

Table 4: Wyckoff bond: `12d@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	$[-X,\ -Y,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[4]`
5	$[Y,\ -X+Y,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[5]`
6	$[X-Y,\ X,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[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]`

continued ...

Table 4

No.	vector	center	mapping
10	$[Y,\, X,\, Z]$	$\left[0,\, 0,\, z+\frac{1}{2}\right]$	`[10]`
11	$[X-Y,\, -Y,\, Z]$	$\left[0,\, 0,\, z+\frac{1}{2}\right]$	`[11]`
12	$[-X,\, -X+Y,\, Z]$	$\left[0,\, 0,\, z+\frac{1}{2}\right]$	`[12]`

* Wyckoff site: `2b`, site symmetry: `3m.`

Table 5: Wyckoff bond: `2a@2b`

No.	vector	center	mapping
1	$[0,\, 0,\, Z]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[1,2,3,7,8,9]`
2	$[0,\, 0,\, Z]$	$\left[\frac{2}{3},\, \frac{1}{3},\, z+\frac{1}{2}\right]$	`[4,5,6,10,11,12]`

Table 6: Wyckoff bond: `6b@2b`

No.	vector	center	mapping
1	$[X,\, 2X,\, Z]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[1,8]`
2	$[-2X,\, -X,\, Z]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[2,7]`
3	$[X,\, -X,\, Z]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[3,9]`
4	$[-X,\, -2X,\, Z]$	$\left[\frac{2}{3},\, \frac{1}{3},\, z+\frac{1}{2}\right]$	`[4,11]`
5	$[2X,\, X,\, Z]$	$\left[\frac{2}{3},\, \frac{1}{3},\, z+\frac{1}{2}\right]$	`[5,10]`
6	$[-X,\, X,\, Z]$	$\left[\frac{2}{3},\, \frac{1}{3},\, z+\frac{1}{2}\right]$	`[6,12]`

Table 7: Wyckoff bond: `6c@2b`

No.	vector	center	mapping
1	$[X,\, 0,\, 0]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[1,-8]`
2	$[0,\, X,\, 0]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[2,-7]`
3	$[-X,\, -X,\, 0]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[3,-9]`
4	$[-X,\, 0,\, 0]$	$\left[\frac{2}{3},\, \frac{1}{3},\, z+\frac{1}{2}\right]$	`[4,-11]`
5	$[0,\, -X,\, 0]$	$\left[\frac{2}{3},\, \frac{1}{3},\, z+\frac{1}{2}\right]$	`[5,-10]`
6	$[X,\, X,\, 0]$	$\left[\frac{2}{3},\, \frac{1}{3},\, z+\frac{1}{2}\right]$	`[6,-12]`

Table 8: Wyckoff bond: `12d@2b`

No.	vector	center	mapping
1	$[X,\, Y,\, Z]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[1]`
2	$[-Y,\, X-Y,\, Z]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[2]`
3	$[-X+Y,\, -X,\, Z]$	$\left[\frac{1}{3},\, \frac{2}{3},\, z\right]$	`[3]`

continued ...

Table 8

No.	vector	center	mapping
4	$[-X, -Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[4]`
5	$[Y, -X+Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[5]`
6	$[X-Y, X, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[6]`
7	$[-Y, -X, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, z\right]$	`[7]`
8	$[-X+Y, Y, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, z\right]$	`[8]`
9	$[X, X-Y, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, z\right]$	`[9]`
10	$[Y, X, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[10]`
11	$[X-Y, -Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[11]`
12	$[-X, -X+Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[12]`

* Wyckoff site: `6c`, site symmetry: `.m.`

Table 9: 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	$[-X, X, Z]$	$\left[-x, x, z+\frac{1}{2}\right]$	`[4,10]`
5	$[-X, -2X, Z]$	$\left[-x, -2x, z+\frac{1}{2}\right]$	`[5,12]`
6	$[2X, X, Z]$	$\left[2x, x, z+\frac{1}{2}\right]$	`[6,11]`

Table 10: 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	$[-X, -X, 0]$	$\left[-x, x, z+\frac{1}{2}\right]$	`[4,-10]`
5	$[X, 0, 0]$	$\left[-x, -2x, z+\frac{1}{2}\right]$	`[5,-12]`
6	$[0, X, 0]$	$\left[2x, x, z+\frac{1}{2}\right]$	`[6,-11]`

Table 11: 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	$[-X, -Y, Z]$	$\left[-x, x, z+\frac{1}{2}\right]$	`[4]`
5	$[Y, -X+Y, Z]$	$\left[-x, -2x, z+\frac{1}{2}\right]$	`[5]`

continued ...

Table 11

No.	vector	center	mapping
6	$[X-Y,\, X,\, Z]$	$\left[2x,\, x,\, z+\frac{1}{2}\right]$	[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	$[Y,\, X,\, Z]$	$\left[-x,\, x,\, z+\frac{1}{2}\right]$	[10]
11	$[X-Y,\, -Y,\, Z]$	$\left[2x,\, x,\, z+\frac{1}{2}\right]$	[11]
12	$[-X,\, -X+Y,\, Z]$	$\left[-x,\, -2x,\, z+\frac{1}{2}\right]$	[12]

* Wyckoff site: 12d, site symmetry: 1

Table 12: 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	$[-X,\, -Y,\, Z]$	$\left[-x,\, -y,\, z+\frac{1}{2}\right]$	[4]
5	$[Y,\, -X+Y,\, Z]$	$\left[y,\, -x+y,\, z+\frac{1}{2}\right]$	[5]
6	$[X-Y,\, X,\, Z]$	$\left[x-y,\, x,\, z+\frac{1}{2}\right]$	[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	$[Y,\, X,\, Z]$	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[10]
11	$[X-Y,\, -Y,\, Z]$	$\left[x-y,\, -y,\, z+\frac{1}{2}\right]$	[11]
12	$[-X,\, -X+Y,\, Z]$	$\left[-x,\, -x+y,\, z+\frac{1}{2}\right]$	[12]