SG No. 185 C_{6v}^3 $P6_3cm$ [hexagonal]

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

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

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

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

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

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

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

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	$[-Y,\ -X,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[7]`
8	$[-X+Y,\ Y,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[8]`
9	$[X,\ X-Y,\ Z]$	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[9]`

continued ...

Table 4

No.	vector	center	mapping
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: `4b`, site symmetry: `3..`

Table 5: Wyckoff bond: `4a@4b`

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

Table 6: Wyckoff bond: `12b@4b`

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]`
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	$[-Y, -X, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, z+\frac{1}{2}\right]$	`[7]`
8	$[-X+Y, Y, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, z+\frac{1}{2}\right]$	`[8]`
9	$[X, X-Y, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, z+\frac{1}{2}\right]$	`[9]`
10	$[Y, X, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z\right]$	`[10]`
11	$[X-Y, -Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z\right]$	`[11]`
12	$[-X, -X+Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z\right]$	`[12]`

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

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

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

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

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

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

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