SG No. 176 C_{6h}^2 $P6_3/m$ [hexagonal]

* plus set: $+[0,\ 0,\ 0]$
* Wyckoff site: `2a`, site symmetry: `-6..`

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

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

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

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

Table 3: Wyckoff bond: `12c@2a`

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

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

Table 4: Wyckoff bond: `2a@2b`

No.	vector	center	mapping
1	$[0,\ 0,\ Z]$	$[0,\ 0,\ 0]$	`[1,2,3,-7,-8,-9]`

continued ...

Table 4

No.	vector	center	mapping
2	$[0, 0, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[4,5,6,-10,-11,-12]`

Table 5: Wyckoff bond: `6b@2b`

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

* Wyckoff site: `2c`, site symmetry: `-6..`

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

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

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

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

Table 8: Wyckoff bond: `12c@2c`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\right]$	`[1]`
2	$[-Y, X-Y, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\right]$	`[2]`
3	$[-X+Y, -X, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}\right]$	`[3]`
4	$[-X, -Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\right]$	`[4]`
5	$[Y, -X+Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}\right]$	`[5]`

continued ...

Table 8

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

* Wyckoff site: `2d`, site symmetry: `-6..`

Table 9: Wyckoff bond: `2a@2d`

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

Table 10: Wyckoff bond: `6b@2d`

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

Table 11: Wyckoff bond: `12c@2d`

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

continued ...

Table 11

No.	vector	center	mapping
12	$[-X+Y,\ -X,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{4}\right]$	`[12]`

* Wyckoff site: `4e`, site symmetry: `3..`

Table 12: Wyckoff bond: `4a@4e`

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

Table 13: Wyckoff bond: `12b@4e`

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	$[-X,\ -Y,\ -Z]$	$[0,\ 0,\ -z]$	`[7]`
8	$[Y,\ -X+Y,\ -Z]$	$[0,\ 0,\ -z]$	`[8]`
9	$[X-Y,\ X,\ -Z]$	$[0,\ 0,\ -z]$	`[9]`
10	$[X,\ Y,\ -Z]$	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	`[10]`
11	$[-Y,\ X-Y,\ -Z]$	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	`[11]`
12	$[-X+Y,\ -X,\ -Z]$	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	`[12]`

* Wyckoff site: `4f`, site symmetry: `3..`

Table 14: Wyckoff bond: `4a@4f`

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	$[0,\ 0,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$	`[7,8,9]`
4	$[0,\ 0,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}-z\right]$	`[10,11,12]`

Table 15: Wyckoff bond: `12b@4f`

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

* Wyckoff site: `6g`, site symmetry: `-1`

Table 16: Wyckoff bond: `6a@6g`

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

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

Table 17: Wyckoff bond: `6a@6h`

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

Table 18: Wyckoff bond: `6b@6h`

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

Table 19: Wyckoff bond: `12c@6h`

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

* Wyckoff site: `12i`, site symmetry: `1`

Table 20: Wyckoff bond: `12a@12i`

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