SG No. 190 D_{3h}^4 $P\bar{6}2c$ [hexagonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `2a`, site symmetry: `32.`

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

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

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

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

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

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

Table 4: Wyckoff bond: `12d@2a`

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

continued ...

Table 4

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

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

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

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

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

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

Table 7: Wyckoff bond: `12c@2b`

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

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

Table 8: 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,-4,-5,-6]`
2	$[0,\ 0,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[7,8,9,-10,-11,-12]`

Table 9: Wyckoff bond: `6b@2c`

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

Table 10: 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	$[X,\ Y,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{4}\right]$	`[4]`
5	$[-Y,\ X-Y,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{4}\right]$	`[5]`
6	$[-X+Y,\ -X,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{4}\right]$	`[6]`
7	$[Y,\ X,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[7]`
8	$[X-Y,\ -Y,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[8]`
9	$[-X,\ -X+Y,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[9]`
10	$[Y,\ X,\ Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[10]`
11	$[X-Y,\ -Y,\ Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[11]`
12	$[-X,\ -X+Y,\ Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	`[12]`

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

Table 11: Wyckoff bond: `2a@2d`

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

Table 12: Wyckoff bond: `6b@2d`

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

Table 13: Wyckoff bond: `12c@2d`

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

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

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

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

Table 15: 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]`

continued ...

Table 15

No.	vector	center	mapping
4	$[X, Y, -Z]$	$\left[0, 0, \frac{1}{2} - z\right]$	[4]
5	$[-Y, X - Y, -Z]$	$\left[0, 0, \frac{1}{2} - z\right]$	[5]
6	$[-X + Y, -X, -Z]$	$\left[0, 0, \frac{1}{2} - z\right]$	[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]
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: 4f, site symmetry: 3..

Table 16: 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	$[0, 0, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z\right]$	[4,5,6]
3	$[0, 0, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	[7,8,9]
4	$[0, 0, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}\right]$	[10,11,12]

Table 17: 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	$[X, Y, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z\right]$	[4]
5	$[-Y, X - Y, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z\right]$	[5]
6	$[-X + Y, -X, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z\right]$	[6]
7	$[Y, X, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	[7]
8	$[X - Y, -Y, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	[8]
9	$[-X, -X + Y, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	[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: 6g, site symmetry: .2.

Table 18: Wyckoff bond: `6a@6g`

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

Table 19: Wyckoff bond: `6b@6g`

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

Table 20: Wyckoff bond: `12c@6g`

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

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

Table 21: Wyckoff bond: `6a@6h`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[x, y, \frac{1}{4}\right]$	`[1,4]`

continued ...

Table 21

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

Table 22: Wyckoff bond: `6b@6h`

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

Table 23: 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	$[X,\ Y,\ -Z]$	$\left[x,\ y,\ \frac{1}{4}\right]$	`[4]`
5	$[-Y,\ X-Y,\ -Z]$	$\left[-y,\ x-y,\ \frac{1}{4}\right]$	`[5]`
6	$[-X+Y,\ -X,\ -Z]$	$\left[-x+y,\ -x,\ \frac{1}{4}\right]$	`[6]`
7	$[Y,\ X,\ -Z]$	$\left[y,\ x,\ \frac{3}{4}\right]$	`[7]`
8	$[X-Y,\ -Y,\ -Z]$	$\left[x-y,\ -y,\ \frac{3}{4}\right]$	`[8]`
9	$[-X,\ -X+Y,\ -Z]$	$\left[-x,\ -x+y,\ \frac{3}{4}\right]$	`[9]`
10	$[Y,\ X,\ Z]$	$\left[y,\ x,\ \frac{3}{4}\right]$	`[10]`
11	$[X-Y,\ -Y,\ Z]$	$\left[x-y,\ -y,\ \frac{3}{4}\right]$	`[11]`
12	$[-X,\ -X+Y,\ Z]$	$\left[-x,\ -x+y,\ \frac{3}{4}\right]$	`[12]`

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

Table 24: 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]`

continued ...

Table 24

No.	vector	center	mapping
4	$[X,\, Y,\, -Z]$	$\left[x,\, y,\, \frac{1}{2}-z\right]$	[4]
5	$[-Y,\, X-Y,\, -Z]$	$\left[-y,\, x-y,\, \frac{1}{2}-z\right]$	[5]
6	$[-X+Y,\, -X,\, -Z]$	$\left[-x+y,\, -x,\, \frac{1}{2}-z\right]$	[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]