SG No. 189 D_{3h}^{3} $P\bar{6}2m$ [hexagonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `-62m`

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

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

Table 2: Wyckoff bond: `3b@1a`

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

Table 3: Wyckoff bond: `3c@1a`

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

Table 4: Wyckoff bond: `6d@1a`

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

Table 5: Wyckoff bond: `6e@1a`

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]`

continued ...

Table 5

No.	vector	center	mapping
4	$[X, 2X, -Z]$	[0, 0, 0]	`[4,-11]`
5	$[-2X, -X, -Z]$	[0, 0, 0]	`[5,-10]`
6	$[X, -X, -Z]$	[0, 0, 0]	`[6,-12]`

Table 6: Wyckoff bond: `6f@1a`

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

Table 7: Wyckoff bond: `12g@1a`

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, 0]	`[4]`
5	$[-Y, X-Y, -Z]$	[0, 0, 0]	`[5]`
6	$[-X+Y, -X, -Z]$	[0, 0, 0]	`[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]`
10	$[Y, X, Z]$	[0, 0, 0]	`[10]`
11	$[X-Y, -Y, Z]$	[0, 0, 0]	`[11]`
12	$[-X, -X+Y, Z]$	[0, 0, 0]	`[12]`

* Wyckoff site: `1b`, site symmetry: `-62m`

Table 8: Wyckoff bond: `1a@1b`

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

Table 9: Wyckoff bond: `3b@1b`

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

Table 10: Wyckoff bond: `3c@1b`

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

Table 11: Wyckoff bond: `6d@1b`

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

Table 12: Wyckoff bond: `6e@1b`

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

Table 13: Wyckoff bond: `6f@1b`

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

continued ...

Table 13

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

Table 14: Wyckoff bond: `12g@1b`

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

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

Table 15: Wyckoff bond: `2a@2c`

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

Table 16: Wyckoff bond: `6b@2c`

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

Table 17: Wyckoff bond: `12c@2c`

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

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

Table 18: Wyckoff bond: `2a@2d`

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

Table 19: Wyckoff bond: `6b@2d`

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

Table 20: Wyckoff bond: `12c@2d`

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

continued ...

Table 20

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

* Wyckoff site: 2e, site symmetry: 3.m

Table 21: Wyckoff bond: 2a@2e

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

Table 22: Wyckoff bond: 6b@2e

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	$[X, 0, -Z]$	$[0, 0, -z]$	[4,8]
5	$[0, X, -Z]$	$[0, 0, -z]$	[5,7]
6	$[-X, -X, -Z]$	$[0, 0, -z]$	[6,9]

Table 23: Wyckoff bond: 6c@2e

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	$[X, 2X, 0]$	$[0, 0, -z]$	[4,-8]
5	$[-2X, -X, 0]$	$[0, 0, -z]$	[5,-7]
6	$[X, -X, 0]$	$[0, 0, -z]$	[6,-9]

Table 24: Wyckoff bond: `12d@2e`

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: `3f`, site symmetry: `m2m`

Table 25: Wyckoff bond: `3a@3f`

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

Table 26: Wyckoff bond: `3b@3f`

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

Table 27: Wyckoff bond: `3c@3f`

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

Table 28: Wyckoff bond: `6d@3f`

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

Table 29: Wyckoff bond: `6e@3f`

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	$[X, 2X, -Z]$	$[x, 0, 0]$	`[4,-11]`
5	$[-2X, -X, -Z]$	$[0, x, 0]$	`[5,-10]`
6	$[X, -X, -Z]$	$[-x, -x, 0]$	`[6,-12]`

Table 30: Wyckoff bond: `6f@3f`

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

Table 31: Wyckoff bond: `12g@3f`

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]`

continued ...

Table 31

No.	vector	center	mapping
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: `3g`, site symmetry: `m2m`

Table 32: Wyckoff bond: `3a@3g`

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

Table 33: Wyckoff bond: `3b@3g`

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

Table 34: Wyckoff bond: `3c@3g`

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

Table 35: Wyckoff bond: `6d@3g`

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

Table 36: Wyckoff bond: `6e@3g`

No.	vector	center	mapping
1	$[X,\ 2X,\ Z]$	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[1,-8]`
2	$[-2X,\ -X,\ Z]$	$\left[0,\ x,\ \frac{1}{2}\right]$	`[2,-7]`
3	$[X,\ -X,\ Z]$	$\left[-x,\ -x,\ \frac{1}{2}\right]$	`[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 37: Wyckoff bond: `6f@3g`

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

Table 38: Wyckoff bond: `12g@3g`

No.	vector	center	mapping
1	$[X,\ Y,\ Z]$	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[1]`
2	$[-Y,\ X-Y,\ Z]$	$\left[0,\ x,\ \frac{1}{2}\right]$	`[2]`
3	$[-X+Y,\ -X,\ Z]$	$\left[-x,\ -x,\ \frac{1}{2}\right]$	`[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	$[Y,\ X,\ -Z]$	$\left[0,\ x,\ \frac{1}{2}\right]$	`[7]`
8	$[X-Y,\ -Y,\ -Z]$	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[8]`
9	$[-X,\ -X+Y,\ -Z]$	$\left[-x,\ -x,\ \frac{1}{2}\right]$	`[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: `4h`, site symmetry: `3..`

Table 39: Wyckoff bond: `4a@4h`

No.	vector	center	mapping
1	$[0,\ 0,\ Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ z\right]$	`[1,2,3]`

continued ...

Table 39

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

Table 40: Wyckoff bond: `12b@4h`

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	$[X,\ Y,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ -z\right]$	`[4]`
5	$[-Y,\ X-Y,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ -z\right]$	`[5]`
6	$[-X+Y,\ -X,\ -Z]$	$\left[\frac{1}{3},\ \frac{2}{3},\ -z\right]$	`[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	$[Y,\ X,\ Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ z\right]$	`[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: `6i`, site symmetry: `..m`

Table 41: Wyckoff bond: `6a@6i`

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	$[X,\ 0,\ -Z]$	$[x,\ 0,\ -z]$	`[4,8]`
5	$[0,\ X,\ -Z]$	$[0,\ x,\ -z]$	`[5,7]`
6	$[-X,\ -X,\ -Z]$	$[-x,\ -x,\ -z]$	`[6,9]`

Table 42: Wyckoff bond: `6b@6i`

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	$[X,\ 2X,\ 0]$	$[x,\ 0,\ -z]$	`[4,-8]`
5	$[-2X,\ -X,\ 0]$	$[0,\ x,\ -z]$	`[5,-7]`

continued ...

Table 42

No.	vector	center	mapping
6	$[X, -X, 0]$	$[-x, -x, -z]$	`[6,-9]`

Table 43: Wyckoff bond: `12c@6i`

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	$[X, Y, -Z]$	$[x, 0, -z]$	`[4]`
5	$[-Y, X-Y, -Z]$	$[0, x, -z]$	`[5]`
6	$[-X+Y, -X, -Z]$	$[-x, -x, -z]$	`[6]`
7	$[Y, X, -Z]$	$[0, x, -z]$	`[7]`
8	$[X-Y, -Y, -Z]$	$[x, 0, -z]$	`[8]`
9	$[-X, -X+Y, -Z]$	$[-x, -x, -z]$	`[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: `6j`, site symmetry: `m..`

Table 44: Wyckoff bond: `6a@6j`

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

Table 45: Wyckoff bond: `6b@6j`

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

Table 46: Wyckoff bond: `12c@6j`

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

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

Table 47: Wyckoff bond: `6a@6k`

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

Table 48: Wyckoff bond: `6b@6k`

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

Table 49: Wyckoff bond: `12c@6k`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[x, y, \frac{1}{2}\right]$	`[1]`

continued ...

Table 49

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

* Wyckoff site: 12l, site symmetry: 1

Table 50: Wyckoff bond: 12a@12l

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]
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]