SG No. 187 D_{3h}^{1} $P\bar{6}m2$ [hexagonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `-6m2`

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: `-6m2`

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: `1c`, site symmetry: `-6m2`

Table 15: Wyckoff bond: `1a@1c`

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

Table 16: Wyckoff bond: `3b@1c`

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

Table 17: Wyckoff bond: `3c@1c`

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

Table 18: Wyckoff bond: `6d@1c`

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	$[-Y, -X, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	`[7,10]`
5	$[-X+Y, Y, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	`[8,11]`
6	$[X, X-Y, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, 0\right]$	`[9,12]`

Table 19: Wyckoff bond: `6e@1c`

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

Table 20: Wyckoff bond: `6f@1c`

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

Table 21: Wyckoff bond: `12g@1c`

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

* Wyckoff site: `1d`, site symmetry: `-6m2`

Table 22: Wyckoff bond: `1a@1d`

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

Table 23: Wyckoff bond: `3b@1d`

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

Table 24: Wyckoff bond: `3c@1d`

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

Table 25: Wyckoff bond: `6d@1d`

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	$[-Y, -X, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right]$	`[7,10]`
5	$[-X+Y, Y, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right]$	`[8,11]`
6	$[X, X-Y, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right]$	`[9,12]`

Table 26: Wyckoff bond: `6e@1d`

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

Table 27: Wyckoff bond: `6f@1d`

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

Table 28: Wyckoff bond: `12g@1d`

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]`
6	$[-X+Y, -X, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right]$	`[6]`
7	$[-Y, -X, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right]$	`[7]`
8	$[-X+Y, Y, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right]$	`[8]`
9	$[X, X-Y, Z]$	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}\right]$	`[9]`

continued ...

Table 28

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

* Wyckoff site: `1e`, site symmetry: `-6m2`

Table 29: Wyckoff bond: `1a@1e`

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

Table 30: Wyckoff bond: `3b@1e`

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

Table 31: Wyckoff bond: `3c@1e`

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

Table 32: Wyckoff bond: `6d@1e`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[1,4]`
2	$[-Y, X-Y, 0]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[2,5]`
3	$[-X+Y, -X, 0]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[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 33: Wyckoff bond: `6e@1e`

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

Table 34: Wyckoff bond: `6f@1e`

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

Table 35: Wyckoff bond: `12g@1e`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[1]`
2	$[-Y, X-Y, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[2]`
3	$[-X+Y, -X, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[3]`
4	$[X, Y, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[4]`
5	$[-Y, X-Y, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[5]`
6	$[-X+Y, -X, -Z]$	$\left[\frac{2}{3}, \frac{1}{3}, 0\right]$	`[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: `1f`, site symmetry: `-6m2`

Table 36: Wyckoff bond: `1a@1f`

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

Table 37: Wyckoff bond: `3b@1f`

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

Table 38: Wyckoff bond: `3c@1f`

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

Table 39: Wyckoff bond: `6d@1f`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}\right]$	`[1,4]`
2	$[-Y, X-Y, 0]$	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}\right]$	`[2,5]`
3	$[-X+Y, -X, 0]$	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}\right]$	`[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 40: Wyckoff bond: `6e@1f`

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

Table 41: Wyckoff bond: `6f@1f`

No.	vector	center	mapping
1	$[X, 0, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}\right]$	`[1,-11]`
2	$[0, X, Z]$	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}\right]$	`[2,-10]`

continued ...

Table 41

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

Table 42: Wyckoff bond: `12g@1f`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	`[1]`
2	$[-Y, X-Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	`[2]`
3	$[-X+Y, -X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	`[3]`
4	$[X, Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	`[4]`
5	$[-Y, X-Y, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	`[5]`
6	$[-X+Y, -X, -Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	`[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: `2g`, site symmetry: `3m.`

Table 43: Wyckoff bond: `2a@2g`

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

Table 44: Wyckoff bond: `6b@2g`

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

Table 45: Wyckoff bond: `6c@2g`

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	$[X, 0, 0]$	$[0, 0, -z]$	`[4,-11]`
5	$[0, X, 0]$	$[0, 0, -z]$	`[5,-10]`
6	$[-X, -X, 0]$	$[0, 0, -z]$	`[6,-12]`

Table 46: Wyckoff bond: `12d@2g`

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: `2h`, site symmetry: `3m.`

Table 47: Wyckoff bond: `2a@2h`

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

Table 48: Wyckoff bond: `6b@2h`

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	$[X, 2X, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[4,11]`
5	$[-2X, -X, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[5,10]`

continued ...

Table 48

No.	vector	center	mapping
6	$[X, -X, -Z]$	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[6,12]`

Table 49: Wyckoff bond: `6c@2h`

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	$[X, 0, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[4,-11]`
5	$[0, X, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[5,-10]`
6	$[-X, -X, 0]$	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[6,-12]`

Table 50: Wyckoff bond: `12d@2h`

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

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

Table 51: Wyckoff bond: `2a@2i`

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

Table 52: Wyckoff bond: `6b@2i`

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

Table 53: Wyckoff bond: `6c@2i`

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

Table 54: Wyckoff bond: `12d@2i`

No.	vector	center	mapping
1	$[X,\ Y,\ Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ z\right]$	`[1]`
2	$[-Y,\ X-Y,\ Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ z\right]$	`[2]`
3	$[-X+Y,\ -X,\ Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ z\right]$	`[3]`
4	$[X,\ Y,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$	`[4]`
5	$[-Y,\ X-Y,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$	`[5]`
6	$[-X+Y,\ -X,\ -Z]$	$\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$	`[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: `3j`, site symmetry: `mm2`

Table 55: Wyckoff bond: `3a@3j`

No.	vector	center	mapping
1	$[X,\ -X,\ 0]$	$[x,\ -x,\ 0]$	`[1,4,7,10]`

continued ...

Table 55

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

Table 56: Wyckoff bond: `3b@3j`

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

Table 57: Wyckoff bond: `3c@3j`

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

Table 58: Wyckoff bond: `6d@3j`

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

Table 59: Wyckoff bond: `6e@3j`

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

Table 60: Wyckoff bond: `6f@3j`

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

Table 61: Wyckoff bond: `12g@3j`

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

* Wyckoff site: `3k`, site symmetry: `mm2`

Table 62: Wyckoff bond: `3a@3k`

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

Table 63: Wyckoff bond: `3b@3k`

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

Table 64: Wyckoff bond: `3c@3k`

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

Table 65: Wyckoff bond: `6d@3k`

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

Table 66: Wyckoff bond: `6e@3k`

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

Table 67: Wyckoff bond: `6f@3k`

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

Table 68: Wyckoff bond: `12g@3k`

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

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

Table 69: Wyckoff bond: `6a@6l`

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 70: Wyckoff bond: `6b@6l`

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 71: Wyckoff bond: `12c@6l`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, 0]$	`[1]`

continued ...

Table 71

No.	vector	center	mapping
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: `6m`, site symmetry: `m..`

Table 72: Wyckoff bond: `6a@6m`

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 73: Wyckoff bond: `6b@6m`

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 74: Wyckoff bond: `12c@6m`

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

continued ...

Table 74

No.	vector	center	mapping
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: `6n`, site symmetry: `.m.`

Table 75: Wyckoff bond: `6a@6n`

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

Table 76: Wyckoff bond: `6b@6n`

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

Table 77: Wyckoff bond: `12c@6n`

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	$[X,\ Y,\ -Z]$	$[x,\ -x,\ -z]$	`[4]`
5	$[-Y,\ X-Y,\ -Z]$	$[x,\ 2x,\ -z]$	`[5]`

continued ...

Table 77

No.	vector	center	mapping
6	$[-X+Y, -X, -Z]$	$[-2x, -x, -z]$	[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	$[-Y, -X, -Z]$	$[x, -x, -z]$	[10]
11	$[-X+Y, Y, -Z]$	$[-2x, -x, -z]$	[11]
12	$[X, X-Y, -Z]$	$[x, 2x, -z]$	[12]

* Wyckoff site: 12o, site symmetry: 1

Table 78: Wyckoff bond: 12a@12o

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]