SG No. 180 D_6^4 $P6_222$ [hexagonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `3a`, site symmetry: `222`

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

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

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

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

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

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

Table 4: Wyckoff bond: `6d@3a`

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

Table 5: Wyckoff bond: `6e@3a`

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[0, 0, 0]$	`[1,-8]`

continued ...

Table 5

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

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

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

Table 7: Wyckoff bond: `12g@3a`

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

* Wyckoff site: `3b`, site symmetry: `222`

Table 8: Wyckoff bond: `3a@3b`

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

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

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

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

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

Table 11: Wyckoff bond: `6d@3b`

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

Table 12: Wyckoff bond: `6e@3b`

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

Table 13: Wyckoff bond: `6f@3b`

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

Table 14: Wyckoff bond: `12g@3b`

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

* Wyckoff site: `3c`, site symmetry: `222`

Table 15: Wyckoff bond: `3a@3c`

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

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

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

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

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

Table 18: Wyckoff bond: `6d@3c`

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

Table 19: Wyckoff bond: `6e@3c`

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

Table 20: Wyckoff bond: `6f@3c`

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

Table 21: Wyckoff bond: `12g@3c`

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

* Wyckoff site: `3d`, site symmetry: `222`

Table 22: Wyckoff bond: `3a@3d`

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

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

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

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

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

Table 25: Wyckoff bond: `6d@3d`

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

Table 26: Wyckoff bond: `6e@3d`

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

Table 27: Wyckoff bond: `6f@3d`

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

Table 28: Wyckoff bond: `12g@3d`

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

continued ...

Table 28

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

* Wyckoff site: `6e`, site symmetry: `2..`

Table 29: Wyckoff bond: `6a@6e`

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

Table 30: Wyckoff bond: `6b@6e`

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

Table 31: Wyckoff bond: `12c@6e`

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

continued ...

Table 31

No.	vector	center	mapping
12	$[X,\ X-Y,\ -Z]$	$\left[0,\ 0,\ \frac{1}{3}-z\right]$	`[12]`

* Wyckoff site: `6f`, site symmetry: `2..`

Table 32: Wyckoff bond: `6a@6f`

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

Table 33: Wyckoff bond: `6b@6f`

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

Table 34: Wyckoff bond: `12c@6f`

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

* Wyckoff site: 6g, site symmetry: .2.

Table 35: Wyckoff bond: 6a@6g

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

Table 36: Wyckoff bond: 6b@6g

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

Table 37: Wyckoff bond: 12c@6g

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

* Wyckoff site: 6h, site symmetry: .2.

Table 38: Wyckoff bond: `6a@6h`

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

Table 39: Wyckoff bond: `6b@6h`

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

Table 40: Wyckoff bond: `12c@6h`

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

* Wyckoff site: `6i`, site symmetry: `..2`

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

No.	vector	center	mapping
1	$[X,\ 0,\ Z]$	$[x,\ 2x,\ 0]$	`[1,-11]`

continued ...

Table 41

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

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

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

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

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

* Wyckoff site: `6j`, site symmetry: `..2`

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

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

continued ...

Table 44

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

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

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

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

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

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

Table 47: Wyckoff bond: `12a@12k`

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

continued ...

Table 47

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