SG No. 181 D_6^5 $P6_422$ [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	$[-2X, -X, 0]$	$\left[0, 0, \frac{1}{3}\right]$	[2,-5,-7,10]
3	$[X, -X, 0]$	$\left[0, 0, \frac{2}{3}\right]$	[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	$[0, X, 0]$	$\left[0, 0, \frac{1}{3}\right]$	[2,-5,7,-10]
3	$[-X, -X, 0]$	$\left[0, 0, \frac{2}{3}\right]$	[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	$[0, 0, Z]$	$\left[0, 0, \frac{1}{3}\right]$	[2,5,-7,-10]
3	$[0, 0, Z]$	$\left[0, 0, \frac{2}{3}\right]$	[3,6,-9,-12]

Table 4: Wyckoff bond: 6d@3a

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

Table 5: Wyckoff bond: 6e@3a

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

continued …

1

Table 5

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

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

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

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

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

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

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

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

Table 28

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

Table 30: Wyckoff bond: 6b@6e

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

Table 31: Wyckoff bond: 12c@6e

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

Table 31

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

Table 36: Wyckoff bond: `6b@6g`

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

Table 37: Wyckoff bond: `12c@6g`

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

Table 42: Wyckoff bond: 6b@6i

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

Table 43: Wyckoff bond: 12c@6i

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

continued ...

Table 44

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

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

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

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

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

continued …

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Table 47

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