SG No. 195 T^1 $P23$ [cubic]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `23.`

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

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

Table 2: Wyckoff bond: `4b@1a`

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

Table 3: Wyckoff bond: `6c@1a`

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

Table 4: Wyckoff bond: `12d@1a`

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

continued ...

Table 4

No.	vector	center	mapping
11	$[Y, -Z, -X]$	[0, 0, 0]	`[11]`
12	$[-Y, -Z, X]$	[0, 0, 0]	`[12]`

* Wyckoff site: `1b`, site symmetry: `23.`

Table 5: Wyckoff bond: `3a@1b`

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

Table 6: Wyckoff bond: `4b@1b`

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

Table 7: Wyckoff bond: `6c@1b`

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

Table 8: Wyckoff bond: `12d@1b`

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

continued ...

Table 8

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

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

Table 9: Wyckoff bond: `3a@3c`

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

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

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

Table 11: Wyckoff bond: `3c@3c`

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

Table 12: Wyckoff bond: `6d@3c`

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

continued ...

Table 12

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

Table 13: Wyckoff bond: `6e@3c`

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

Table 14: Wyckoff bond: `6f@3c`

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

Table 15: Wyckoff bond: `12g@3c`

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

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

Table 16: Wyckoff bond: 3a@3d

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

Table 17: Wyckoff bond: 3b@3d

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

Table 18: Wyckoff bond: 3c@3d

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

Table 19: Wyckoff bond: 6d@3d

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

Table 20: Wyckoff bond: 6e@3d

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

continued ...

Table 20

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

Table 21: Wyckoff bond: `6f@3d`

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

Table 22: Wyckoff bond: `12g@3d`

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

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

Table 23: Wyckoff bond: `4a@4e`

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

Table 24: Wyckoff bond: `12b@4e`

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

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

Table 25: Wyckoff bond: `6a@6f`

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

Table 26: Wyckoff bond: `6b@6f`

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

Table 27: Wyckoff bond: `12c@6f`

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

continued ...

Table 27

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

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

Table 28: Wyckoff bond: `6a@6g`

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

Table 29: Wyckoff bond: `6b@6g`

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

Table 30: Wyckoff bond: `12c@6g`

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

continued ...

Table 30

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

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

Table 31: Wyckoff bond: `6a@6h`

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

Table 32: Wyckoff bond: `6b@6h`

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

Table 33: Wyckoff bond: `12c@6h`

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

continued ...

Table 33

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

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

Table 34: Wyckoff bond: 6a@6i

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

Table 35: Wyckoff bond: 6b@6i

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

Table 36: Wyckoff bond: 12c@6i

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

continued ...

Table 36

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

* Wyckoff site: 12j, site symmetry: 1

Table 37: Wyckoff bond: 12a@12j

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