SG No. 112 D_{2d}^2 $P\bar{4}2c$ [tetragonal]

* plus set: $+[0, 0, 0]$

* Wyckoff site: 2a, site symmetry: 222.

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 2b@2a

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

Table 3: Wyckoff bond: 2c@2a

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

Table 4: Wyckoff bond: 4d@2a

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

Table 5: Wyckoff bond: 4e@2a

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

Table 6: Wyckoff bond: `4f@2a`

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

Table 7: Wyckoff bond: `8g@2a`

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

* Wyckoff site: `2b`, site symmetry: `222`.

Table 8: Wyckoff bond: `2a@2b`

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

Table 9: Wyckoff bond: `2b@2b`

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

Table 10: Wyckoff bond: `2c@2b`

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

Table 11: Wyckoff bond: `4d@2b`

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

Table 12: Wyckoff bond: `4e@2b`

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

Table 13: Wyckoff bond: `4f@2b`

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

Table 14: Wyckoff bond: `8g@2b`

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

* Wyckoff site: `2c`, site symmetry: `222`.

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

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

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

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

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

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

Table 18: Wyckoff bond: `4d@2c`

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

Table 19: Wyckoff bond: `4e@2c`

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

Table 20: Wyckoff bond: `4f@2c`

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

Table 21: Wyckoff bond: `8g@2c`

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

* Wyckoff site: `2d`, site symmetry: `222`.

Table 22: Wyckoff bond: `2a@2d`

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

Table 23: Wyckoff bond: `2b@2d`

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

Table 24: Wyckoff bond: `2c@2d`

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

Table 25: Wyckoff bond: `4d@2d`

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

Table 26: Wyckoff bond: `4e@2d`

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

Table 27: Wyckoff bond: `4f@2d`

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

Table 28: Wyckoff bond: `8g@2d`

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

* Wyckoff site: `2e`, site symmetry: `-4..`

Table 29: Wyckoff bond: `2a@2e`

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

Table 30: Wyckoff bond: `4b@2e`

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

Table 31: Wyckoff bond: `8c@2e`

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

* Wyckoff site: `2f`, site symmetry: `-4..`

Table 32: Wyckoff bond: `2a@2f`

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

Table 33: Wyckoff bond: `4b@2f`

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

continued ...

Table 33

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

Table 34: Wyckoff bond: 8c@2f

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

* Wyckoff site: 4g, site symmetry: .2.

Table 35: Wyckoff bond: 4a@4g

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

Table 36: Wyckoff bond: 4b@4g

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

Table 37: Wyckoff bond: 8c@4g

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

Table 37

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

* Wyckoff site: 4h, site symmetry: .2.

Table 38: Wyckoff bond: 4a@4h

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

Table 39: Wyckoff bond: 4b@4h

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

Table 40: Wyckoff bond: 8c@4h

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

* Wyckoff site: 4i, site symmetry: .2.

Table 41: Wyckoff bond: `4a@4i`

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

Table 42: Wyckoff bond: `4b@4i`

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

Table 43: Wyckoff bond: `8c@4i`

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

* Wyckoff site: `4j`, site symmetry: `.2.`

Table 44: Wyckoff bond: `4a@4j`

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

Table 45: Wyckoff bond: `4b@4j`

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

Table 46: Wyckoff bond: `8c@4j`

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

* Wyckoff site: `4k`, site symmetry: `2..`

Table 47: Wyckoff bond: `4a@4k`

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

Table 48: Wyckoff bond: `4b@4k`

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

Table 49: Wyckoff bond: `8c@4k`

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

* Wyckoff site: `4l`, site symmetry: `2..`

Table 50: Wyckoff bond: `4a@4l`

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

Table 51: Wyckoff bond: `4b@4l`

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

Table 52: Wyckoff bond: `8c@4l`

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

* Wyckoff site: 4m, site symmetry: 2..

Table 53: Wyckoff bond: 4a@4m

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

Table 54: Wyckoff bond: 4b@4m

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

Table 55: Wyckoff bond: 8c@4m

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

* Wyckoff site: 8n, site symmetry: 1

Table 56: Wyckoff bond: 8a@8n

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

8	$[Y, X, Z]$	$\left[y, x, z + \frac{1}{2}\right]$	[8]