SG No. 111 D_{2d}^{1} $P\bar{4}2m$ [tetragonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `-42m`

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]`

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

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

Table 3: Wyckoff bond: `2c@1a`

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

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

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

Table 5: Wyckoff bond: `4e@1a`

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

Table 6: Wyckoff bond: `4f@1a`

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

Table 7: Wyckoff bond: `8g@1a`

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	$[-X, Y, -Z]$	[0, 0, 0]	`[5]`
6	$[X, -Y, -Z]$	[0, 0, 0]	`[6]`
7	$[-Y, -X, Z]$	[0, 0, 0]	`[7]`
8	$[Y, X, Z]$	[0, 0, 0]	`[8]`

* Wyckoff site: `1b`, site symmetry: `-42m`

Table 8: Wyckoff bond: `1a@1b`

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

Table 9: Wyckoff bond: `2b@1b`

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

Table 10: Wyckoff bond: `2c@1b`

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

Table 11: Wyckoff bond: `4d@1b`

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

Table 12: Wyckoff bond: `4e@1b`

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

Table 13: Wyckoff bond: `4f@1b`

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

Table 14: Wyckoff bond: `8g@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	$[Y, -X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[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: `1c`, site symmetry: `-42m`

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

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

Table 16: Wyckoff bond: `2b@1c`

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

Table 17: Wyckoff bond: `2c@1c`

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

Table 18: Wyckoff bond: `4d@1c`

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

Table 19: Wyckoff bond: `4e@1c`

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

Table 20: Wyckoff bond: `4f@1c`

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

continued ...

Table 20

No.	vector	center	mapping
2	$[Y, -X, 0]$	$\left[0, 0, \frac{1}{2}\right]$	`[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 21: Wyckoff bond: `8g@1c`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[2]`
3	$[Y, -X, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	`[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: `1d`, site symmetry: `-42m`

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

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

Table 23: Wyckoff bond: `2b@1d`

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

Table 24: Wyckoff bond: `2c@1d`

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

Table 25: Wyckoff bond: `4d@1d`

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

Table 26: Wyckoff bond: `4e@1d`

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

Table 27: Wyckoff bond: `4f@1d`

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	$[-X, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[5,-6]`
4	$[-Y, -X, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[7,-8]`

Table 28: Wyckoff bond: `8g@1d`

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	$[-X, Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[5]`
6	$[X, -Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[6]`
7	$[-Y, -X, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[7]`
8	$[Y, X, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[8]`

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

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

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

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

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

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

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

Table 32: Wyckoff bond: `4d@2e`

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

Table 33: Wyckoff bond: `4e@2e`

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

Table 34: Wyckoff bond: `4f@2e`

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

Table 35: Wyckoff bond: `8g@2e`

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	$[Y, -X, -Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[4]`
5	$[-X, Y, -Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[5]`
6	$[X, -Y, -Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[6]`
7	$[-Y, -X, Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[7]`
8	$[Y, X, Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[8]`

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

Table 36: Wyckoff bond: `2a@2f`

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

Table 37: Wyckoff bond: `2b@2f`

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

Table 38: Wyckoff bond: `2c@2f`

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

Table 39: Wyckoff bond: `4d@2f`

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

Table 40: Wyckoff bond: `4e@2f`

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

Table 41: Wyckoff bond: `4f@2f`

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

Table 42: Wyckoff bond: `8g@2f`

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

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

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

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

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

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

Table 45: Wyckoff bond: `4c@2g`

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

Table 46: Wyckoff bond: `4d@2g`

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

Table 47: Wyckoff bond: `8e@2g`

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	$[-X, Y, -Z]$	$[0, 0, -z]$	`[5]`
6	$[X, -Y, -Z]$	$[0, 0, -z]$	`[6]`
7	$[-Y, -X, Z]$	$[0, 0, z]$	`[7]`
8	$[Y, X, Z]$	$[0, 0, z]$	`[8]`

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

Table 48: Wyckoff bond: 2a@2h

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

Table 49: Wyckoff bond: 2b@2h

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

Table 50: Wyckoff bond: 4c@2h

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

Table 51: Wyckoff bond: 4d@2h

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

Table 52: Wyckoff bond: 8e@2h

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

continued ...

Table 52

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

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

Table 53: Wyckoff bond: `4a@4i`

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

Table 54: Wyckoff bond: `4b@4i`

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

Table 55: Wyckoff bond: `8c@4i`

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

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

Table 56: Wyckoff bond: `4a@4j`

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

Table 57: Wyckoff bond: `4b@4j`

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

Table 58: Wyckoff bond: `8c@4j`

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	$[Y,\ -X,\ -Z]$	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[3]`
4	$[-Y,\ X,\ -Z]$	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[4]`
5	$[-X,\ Y,\ -Z]$	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[5]`
6	$[X,\ -Y,\ -Z]$	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[6]`
7	$[-Y,\ -X,\ Z]$	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[7]`
8	$[Y,\ X,\ Z]$	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[8]`

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

Table 59: Wyckoff bond: `4a@4k`

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

Table 60: Wyckoff bond: `4b@4k`

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

Table 61: Wyckoff bond: `8c@4k`

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	$[Y,\ -X,\ -Z]$	$\left[0,\ -x,\ \frac{1}{2}\right]$	`[3]`
4	$[-Y,\ X,\ -Z]$	$\left[0,\ x,\ \frac{1}{2}\right]$	`[4]`
5	$[-X,\ Y,\ -Z]$	$\left[-x,\ 0,\ \frac{1}{2}\right]$	`[5]`
6	$[X,\ -Y,\ -Z]$	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[6]`
7	$[-Y,\ -X,\ Z]$	$\left[0,\ -x,\ \frac{1}{2}\right]$	`[7]`
8	$[Y,\ X,\ Z]$	$\left[0,\ x,\ \frac{1}{2}\right]$	`[8]`

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

Table 62: Wyckoff bond: `4a@4l`

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

Table 63: Wyckoff bond: `4b@4l`

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

Table 64: Wyckoff bond: `8c@4l`

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	$[Y, -X, -Z]$	$\left[\frac{1}{2}, -x, 0\right]$	`[3]`
4	$[-Y, X, -Z]$	$\left[\frac{1}{2}, x, 0\right]$	`[4]`
5	$[-X, Y, -Z]$	$\left[-x, \frac{1}{2}, 0\right]$	`[5]`
6	$[X, -Y, -Z]$	$\left[x, \frac{1}{2}, 0\right]$	`[6]`
7	$[-Y, -X, Z]$	$\left[\frac{1}{2}, -x, 0\right]$	`[7]`
8	$[Y, X, Z]$	$\left[\frac{1}{2}, x, 0\right]$	`[8]`

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

Table 65: 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	$[-X, Y, 0]$	$\left[0, \frac{1}{2}, -z\right]$	`[5,-6]`
4	$[-Y, -X, 0]$	$\left[\frac{1}{2}, 0, z\right]$	`[7,-8]`

Table 66: 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	$[0, 0, -Z]$	$\left[0, \frac{1}{2}, -z\right]$	`[5,6]`
4	$[0, 0, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[7,8]`

Table 67: 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	$[-X, Y, -Z]$	$\left[0, \frac{1}{2}, -z\right]$	`[5]`
6	$[X, -Y, -Z]$	$\left[0, \frac{1}{2}, -z\right]$	`[6]`
7	$[-Y, -X, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[7]`
8	$[Y, X, Z]$	$\left[\frac{1}{2}, 0, z\right]$	`[8]`

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

Table 68: Wyckoff bond: 4a@4n

No.	vector	center	mapping
1	$[X, X, Z]$	$[x, x, z]$	[1,8]
2	$[-X, -X, Z]$	$[-x, -x, z]$	[2,7]
3	$[X, -X, -Z]$	$[x, -x, -z]$	[3,6]
4	$[-X, X, -Z]$	$[-x, x, -z]$	[4,5]

Table 69: Wyckoff bond: 4b@4n

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, z]$	[1,-8]
2	$[-X, X, 0]$	$[-x, -x, z]$	[2,-7]
3	$[-X, -X, 0]$	$[x, -x, -z]$	[3,-6]
4	$[X, X, 0]$	$[-x, x, -z]$	[4,-5]

Table 70: Wyckoff bond: 8c@4n

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

* Wyckoff site: 8o, site symmetry: 1

Table 71: Wyckoff bond: 8a@8o

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	$[-X, Y, -Z]$	$[-x, y, -z]$	[5]
6	$[X, -Y, -Z]$	$[x, -y, -z]$	[6]
7	$[-Y, -X, Z]$	$[-y, -x, z]$	[7]

8	$[Y, X, Z]$	$[y, x, z]$	`[8]`