SG No. 49 D_{2h}^3 $Pccm$ [orthorhombic]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `2a`, site symmetry: `..2/m`

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

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

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

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

Table 3: Wyckoff bond: `4c@2a`

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

* Wyckoff site: `2b`, site symmetry: `..2/m`

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

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

Table 5: Wyckoff bond: `2b@2b`

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

Table 6: Wyckoff bond: `4c@2b`

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

* Wyckoff site: `2c`, site symmetry: `..2/m`

Table 7: Wyckoff bond: `2a@2c`

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

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

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

Table 9: Wyckoff bond: `4c@2c`

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

* Wyckoff site: `2d`, site symmetry: `..2/m`

Table 10: Wyckoff bond: `2a@2d`

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

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

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

Table 12: Wyckoff bond: `4c@2d`

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

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

Table 13: Wyckoff bond: `2a@2e`

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

Table 14: Wyckoff bond: `2b@2e`

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

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

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

Table 16: Wyckoff bond: `4d@2e`

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

Table 17: Wyckoff bond: `4e@2e`

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

Table 18: Wyckoff bond: `4f@2e`

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

Table 19: Wyckoff bond: `8g@2e`

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

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

Table 20: Wyckoff bond: `2a@2f`

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

Table 21: Wyckoff bond: `2b@2f`

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

Table 22: Wyckoff bond: `2c@2f`

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

Table 23: Wyckoff bond: `4d@2f`

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

Table 24: Wyckoff bond: `4e@2f`

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

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

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

Table 26: Wyckoff bond: `8g@2f`

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

* Wyckoff site: `2g`, site symmetry: `222`

Table 27: Wyckoff bond: `2a@2g`

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

Table 28: Wyckoff bond: `2b@2g`

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

Table 29: Wyckoff bond: `2c@2g`

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

Table 30: Wyckoff bond: `4d@2g`

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

Table 31: Wyckoff bond: `4e@2g`

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

Table 32: Wyckoff bond: `4f@2g`

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

Table 33: Wyckoff bond: `8g@2g`

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

* Wyckoff site: `2h`, site symmetry: `222`

Table 34: Wyckoff bond: `2a@2h`

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

Table 35: Wyckoff bond: `2b@2h`

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

Table 36: Wyckoff bond: `2c@2h`

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

Table 37: Wyckoff bond: `4d@2h`

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

Table 38: Wyckoff bond: `4e@2h`

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

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

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

Table 40: Wyckoff bond: `8g@2h`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 65: Wyckoff bond: `4a@4q`

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

Table 66: Wyckoff bond: `4b@4q`

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

Table 67: Wyckoff bond: `8c@4q`

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

* Wyckoff site: `8r`, site symmetry: `1`

Table 68: Wyckoff bond: `8a@8r`

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