SG No. 84 C_{4h}^{2} $P4_2/m$ [tetragonal]

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

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

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

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

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

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

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

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

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

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

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

Table 14: Wyckoff bond: `4b@2e`

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

Table 15: Wyckoff bond: `8c@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	$[-Y,\ X,\ Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[3]`
4	$[Y,\ -X,\ Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[4]`
5	$[-X,\ -Y,\ -Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[5]`
6	$[X,\ Y,\ -Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[6]`
7	$[Y,\ -X,\ -Z]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[7]`

continued ...

Table 15

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

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

Table 16: Wyckoff bond: `2a@2f`

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

Table 17: Wyckoff bond: `4b@2f`

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

Table 18: Wyckoff bond: `8c@2f`

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

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

Table 19: Wyckoff bond: `4a@4g`

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

continued ...

Table 19

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

Table 20: Wyckoff bond: `4b@4g`

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

Table 21: Wyckoff bond: `8c@4g`

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

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

Table 22: Wyckoff bond: `4a@4h`

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

Table 23: Wyckoff bond: `4b@4h`

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

continued ...

Table 23

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

Table 24: Wyckoff bond: `8c@4h`

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

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

Table 25: Wyckoff bond: `4a@4i`

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

Table 26: Wyckoff bond: `4b@4i`

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

Table 27: Wyckoff bond: `8c@4i`

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

continued ...

Table 27

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

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

Table 28: Wyckoff bond: `4a@4j`

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

Table 29: Wyckoff bond: `4b@4j`

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

Table 30: Wyckoff bond: `8c@4j`

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

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

Table 31: Wyckoff bond: `8a@8k`

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