SG No. 85 C_{4h}^{3} $P4/n$ [tetragonal]

* plus set: $+[0,\ 0,\ 0]$
* Wyckoff site: `2a`, site symmetry: `-4..`

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

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

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

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

Table 3: Wyckoff bond: `8c@2a`

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

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

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

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

Table 5: Wyckoff bond: `4b@2b`

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

Table 6: Wyckoff bond: `8c@2b`

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

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

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

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

Table 8: Wyckoff bond: `4b@2c`

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

Table 9: Wyckoff bond: `8c@2c`

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

continued ...

Table 9

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

* Wyckoff site: `4d`, site symmetry: `-1`

Table 10: Wyckoff bond: `4a@4d`

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

* Wyckoff site: `4e`, site symmetry: `-1`

Table 11: Wyckoff bond: `4a@4e`

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

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

Table 12: Wyckoff bond: `4a@4f`

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

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

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

Table 14: Wyckoff bond: `8c@4f`

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

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

Table 15: Wyckoff bond: `8a@8g`

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