SG No. 99 C_{4v}^{1} $P4mm$ [tetragonal]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `1a`, site symmetry: `4mm`

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

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

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

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

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

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

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

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

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

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

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: `1b`, site symmetry: `4mm`

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

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

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

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

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

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

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

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

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

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

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 14: Wyckoff bond: `8g@1b`

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]`
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: `2c`, site symmetry: `2mm.`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 23: Wyckoff bond: `4b@4d`

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 24: Wyckoff bond: `8c@4d`

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: `4e`, site symmetry: `.m.`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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]`