SG No. 100 C_{4v}^{2} $P4bm$ [tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff bond: `4d@2b`

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

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

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

Table 9: Wyckoff bond: `4f@2b`

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

Table 10: Wyckoff bond: `8g@2b`

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	$[X, -Y, Z]$	$\left[0, \frac{1}{2}, z\right]$	`[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: `4c`, site symmetry: `..m`

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

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

Table 12: Wyckoff bond: `4b@4c`

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

Table 13: Wyckoff bond: `8c@4c`

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

* Wyckoff site: 8d, site symmetry: 1

Table 14: Wyckoff bond: 8a@8d

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	$[X, -Y, Z]$	$\left[x + \frac{1}{2}, \frac{1}{2} - y, z\right]$	[5]
6	$[-X, Y, Z]$	$\left[\frac{1}{2} - x, y + \frac{1}{2}, z\right]$	[6]
7	$[-Y, -X, Z]$	$\left[\frac{1}{2} - y, \frac{1}{2} - x, z\right]$	[7]
8	$[Y, X, Z]$	$\left[y + \frac{1}{2}, x + \frac{1}{2}, z\right]$	[8]