SG No. 101 $C_{4\mathrm{v}}^3$ $P4_2cm$ [tetragonal]

* plus set: $+[0, 0, 0]$

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

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

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

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

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

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

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

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

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

Table 5: Wyckoff bond: `8e@2a`

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

continued ...

Table 5

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

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

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

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

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

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

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

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	$[-X, X, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[3,6]
4	$[X, -X, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[4,5]

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

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

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

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	$[X, -Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z+\frac{1}{2}\right]$	[5]
6	$[-X, Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z+\frac{1}{2}\right]$	[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: `4c`, site symmetry: `2..`

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

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

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

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	$[0, 0, Z]$	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	[5,6]
4	$[0, 0, Z]$	$\left[\frac{1}{2}, 0, z\right]$	[7,8]

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

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]
4	$[Y, -X, Z]$	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	[4]
5	$[X, -Y, Z]$	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	[5]
6	$[-X, Y, Z]$	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	[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: `4d`, site symmetry: `..m`

Table 14: 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	$[-X,\,X,\,Z]$	$[-x,\,x,\,z+\frac{1}{2}]$	[3,6]
4	$[X,\,-X,\,Z]$	$[x,\,-x,\,z+\frac{1}{2}]$	[4,5]

Table 15: 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	$[X,\,X,\,0]$	$[-x,\,x,\,z+\frac{1}{2}]$	[3,-6]
4	$[-X,\,-X,\,0]$	$[x,\,-x,\,z+\frac{1}{2}]$	[4,-5]

Table 16: 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	$[-Y,\,X,\,Z]$	$[-x,\,x,\,z+\frac{1}{2}]$	[3]
4	$[Y,\,-X,\,Z]$	$[x,\,-x,\,z+\frac{1}{2}]$	[4]
5	$[X,\,-Y,\,Z]$	$[x,\,-x,\,z+\frac{1}{2}]$	[5]
6	$[-X,\,Y,\,Z]$	$[-x,\,x,\,z+\frac{1}{2}]$	[6]
7	$[-Y,\,-X,\,Z]$	$[-x,\,-x,\,z]$	[7]
8	$[Y,\,X,\,Z]$	$[x,\,x,\,z]$	[8]

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

Table 17: Wyckoff bond: `8a@8e`

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

8	$[Y, X, Z]$	$[y, x, z]$	[8]