SG No. 118 D_{2d}^8 $P\bar{4}n2$ [tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

* Wyckoff site: `2c`, site symmetry: `2.22`

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

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

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

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

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

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

Table 10: Wyckoff bond: 4d@2c

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

Table 11: Wyckoff bond: 4e@2c

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

Table 12: Wyckoff bond: 4f@2c

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

Table 13: Wyckoff bond: 8g@2c

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

* Wyckoff site: 2d, site symmetry: 2.22

Table 14: Wyckoff bond: `2a@2d`

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

Table 15: Wyckoff bond: `2b@2d`

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

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

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

Table 17: Wyckoff bond: `4d@2d`

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

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

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

Table 19: Wyckoff bond: `4f@2d`

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

Table 20: Wyckoff bond: `8g@2d`

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

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

Table 21: Wyckoff bond: `4a@4e`

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

Table 22: Wyckoff bond: `4b@4e`

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

Table 23: Wyckoff bond: 8c@4e

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

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

Table 24: Wyckoff bond: 4a@4f

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

Table 25: Wyckoff bond: 4b@4f

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

Table 26: Wyckoff bond: 8c@4f

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

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

Table 27: Wyckoff bond: 4a@4g

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

Table 28: Wyckoff bond: 4b@4g

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

Table 29: Wyckoff bond: 8c@4g

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

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

Table 30: Wyckoff bond: 4a@4h

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

Table 31: Wyckoff bond: `4b@4h`

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

Table 32: Wyckoff bond: `8c@4h`

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

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

Table 33: Wyckoff bond: `8a@8i`

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