SG No. 109 C_{4v}^{11} $I4_1md$ [tetragonal]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$
* Wyckoff site: `4a`, site symmetry: `2mm.`

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

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

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

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

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

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

Table 4: Wyckoff bond: `8d@4a`

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

Table 5: Wyckoff bond: `8e@4a`

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

Table 6: Wyckoff bond: `8f@4a`

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

Table 7: Wyckoff bond: `16g@4a`

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

* Wyckoff site: `8b`, site symmetry: `.m.`

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

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

Table 9: Wyckoff bond: `8b@8b`

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

Table 10: Wyckoff bond: `16c@8b`

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

* Wyckoff site: `16c`, site symmetry: `1`

Table 11: Wyckoff bond: `16a@16c`

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