SG No. 107 C_{4v}^{9} $I4mm$ [tetragonal]

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

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

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

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

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: `4c@2a`

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: `8d@2a`

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: `8e@2a`

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

Table 6: Wyckoff bond: `8f@2a`

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

Table 7: Wyckoff bond: `16g@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	$[X, -Y, Z]$	$[0, 0, z]$	`[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: `4b`, site symmetry: `2mm`.

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

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

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

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

Table 10: Wyckoff bond: `8c@4b`

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

continued ...

Table 10

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

Table 11: Wyckoff bond: `8d@4b`

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

Table 12: Wyckoff bond: `16e@4b`

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	$[X, -Y, Z]$	$\left[0, \frac{1}{2}, z\right]$	`[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: `8c`, site symmetry: `..m`

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

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 14: Wyckoff bond: `8b@8c`

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]`

continued ...

Table 14

No.	vector	center	mapping
4	$[-X, -X, 0]$	$[x, -x, z]$	`[4,-5]`

Table 15: Wyckoff bond: `16c@8c`

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: `8d`, site symmetry: `.m.`

Table 16: Wyckoff bond: `8a@8d`

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 17: Wyckoff bond: `8b@8d`

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 18: Wyckoff bond: `16c@8d`

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]`

continued ...

Table 18

No.	vector	center	mapping
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: `16e`, site symmetry: `1`

Table 19: Wyckoff bond: `16a@16e`

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]`