SG No. 91 D_4^3 $P4_122$ [tetragonal]

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

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

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

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

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

Table 3: Wyckoff bond: `8c@4a`

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

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

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

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

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

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

Table 6: Wyckoff bond: `8c@4b`

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

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

Table 7: Wyckoff bond: `4a@4c`

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

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

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

Table 9: Wyckoff bond: `8c@4c`

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

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

Table 10: Wyckoff bond: `8a@8d`

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