SG No. 57 D_{2h}^{11} *Pbcm* [orthorhombic]

* plus set: $+[0, 0, 0]$
* Wyckoff site: `4a`, site symmetry: `-1`

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

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

* Wyckoff site: `4b`, site symmetry: `-1`

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

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

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

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

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

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

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

Table 5: Wyckoff bond: `8c@4c`

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

* Wyckoff site: `4d`, site symmetry: `..m`

Table 6: Wyckoff bond: `4a@4d`

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

Table 7: Wyckoff bond: `4b@4d`

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

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

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

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

Table 9: Wyckoff bond: `8a@8e`

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