SG No. 54 D_{2h}^{8} *Pcca* [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	$[-X,\ -Y,\ Z]$	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[2,-6]`
3	$[-X,\ Y,\ -Z]$	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[3,-7]`
4	$[X,\ -Y,\ -Z]$	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[4,-8]`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff bond: `4a@4e`

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

Table 10: Wyckoff bond: `4b@4e`

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

Table 11: Wyckoff bond: `8c@4e`

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

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

Table 12: Wyckoff bond: `8a@8f`

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

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