SG No. 58 D_{2h}^{12} $Pnnm$ [orthorhombic]

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

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

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

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

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

Table 3: Wyckoff bond: `4c@2a`

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

* Wyckoff site: `2b`, site symmetry: `..2/m`

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

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

Table 5: Wyckoff bond: `2b@2b`

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

Table 6: Wyckoff bond: `4c@2b`

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

* Wyckoff site: `2c`, site symmetry: `..2/m`

Table 7: Wyckoff bond: `2a@2c`

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

Table 8: Wyckoff bond: `2b@2c`

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

Table 9: Wyckoff bond: `4c@2c`

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

* Wyckoff site: `2d`, site symmetry: `..2/m`

Table 10: Wyckoff bond: `2a@2d`

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

Table 11: Wyckoff bond: `2b@2d`

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

Table 12: Wyckoff bond: `4c@2d`

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

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

Table 13: Wyckoff bond: `4a@4e`

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

Table 14: Wyckoff bond: `4b@4e`

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

Table 15: Wyckoff bond: `8c@4e`

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

continued ...

Table 15

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

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

Table 16: Wyckoff bond: `4a@4f`

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

Table 17: Wyckoff bond: `4b@4f`

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

Table 18: Wyckoff bond: `8c@4f`

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

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

Table 19: Wyckoff bond: `4a@4g`

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

Table 20: Wyckoff bond: `4b@4g`

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

Table 21: Wyckoff bond: `8c@4g`

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

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

Table 22: Wyckoff bond: `8a@8h`

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