SG No. 59 D_{2h}^{13} $Pmmn$ [orthorhombic]

* plus set: $+[0,\ 0,\ 0]$
* Wyckoff site: `2a`, site symmetry: `mm2`

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

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

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

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

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

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

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

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

Table 5: Wyckoff bond: `4e@2a`

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

Table 6: Wyckoff bond: `4f@2a`

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

Table 7: Wyckoff bond: `8g@2a`

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

* Wyckoff site: `2b`, site symmetry: `mm2`

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

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

Table 9: Wyckoff bond: `2b@2b`

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

Table 10: Wyckoff bond: `2c@2b`

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

Table 11: Wyckoff bond: `4d@2b`

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

Table 12: Wyckoff bond: `4e@2b`

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

Table 13: Wyckoff bond: `4f@2b`

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

Table 14: Wyckoff bond: `8g@2b`

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

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

Table 15: Wyckoff bond: `4a@4c`

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

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

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

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

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

Table 17: Wyckoff bond: `4a@4e`

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

Table 18: Wyckoff bond: `4b@4e`

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

Table 19: Wyckoff bond: `8c@4e`

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

continued ...

Table 19

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

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

Table 20: Wyckoff bond: `4a@4f`

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

Table 21: Wyckoff bond: `4b@4f`

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

Table 22: Wyckoff bond: `8c@4f`

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

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

Table 23: Wyckoff bond: `8a@8g`

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