SG No. 63 D_{2h}^{17} $Cmcm$ [orthorhombic]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$
* Wyckoff site: `4a`, site symmetry: `2/m..`

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

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

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

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

Table 3: Wyckoff bond: `8c@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	$[-X,\ Y,\ -Z]$	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[3,-7]`
4	$[X,\ -Y,\ -Z]$	$[0,\ 0,\ 0]$	`[4,-8]`

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

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

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

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

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

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

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[1,-5]`
2	$[-X, -Y, Z]$	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[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: `4c`, site symmetry: `m2m`

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

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

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

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

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

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

Table 10: Wyckoff bond: `8d@4c`

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

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

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

Table 12: Wyckoff bond: `8f@4c`

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

Table 13: Wyckoff bond: `16g@4c`

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

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

Table 14: Wyckoff bond: `8a@8d`

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

* Wyckoff site: `8e`, site symmetry: `2..`

Table 15: Wyckoff bond: `8a@8e`

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

Table 16: Wyckoff bond: `8b@8e`

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

Table 17: Wyckoff bond: `16c@8e`

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

* Wyckoff site: `8f`, site symmetry: `m..`

Table 18: Wyckoff bond: `8a@8f`

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

Table 19: Wyckoff bond: `8b@8f`

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

Table 20: Wyckoff bond: `16c@8f`

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

* Wyckoff site: `8g`, site symmetry: `..m`

Table 21: Wyckoff bond: `8a@8g`

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	$[-X,\ Y,\ 0]$	$\left[-x,\ y,\ \frac{1}{4}\right]$	`[3,8]`
4	$[X,\ -Y,\ 0]$	$\left[x,\ -y,\ \frac{3}{4}\right]$	`[4,7]`

Table 22: Wyckoff bond: `8b@8g`

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	$[0,\ 0,\ -Z]$	$\left[-x,\ y,\ \frac{1}{4}\right]$	`[3,-8]`
4	$[0,\ 0,\ -Z]$	$\left[x,\ -y,\ \frac{3}{4}\right]$	`[4,-7]`

Table 23: Wyckoff bond: `16c@8g`

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

* Wyckoff site: `16h`, site symmetry: `1`

Table 24: Wyckoff bond: `16a@16h`

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