SG No. 53 D_{2h}^{7} *Pmna* [orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 15

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

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

Table 16: Wyckoff bond: 4a@4f

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

Table 17: Wyckoff bond: 4b@4f

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

Table 18: Wyckoff bond: 8c@4f

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

* Wyckoff site: 4g, site symmetry: .2.

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

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

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

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

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

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

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

Table 22: Wyckoff bond: `4a@4h`

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

Table 23: Wyckoff bond: `4b@4h`

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

Table 24: Wyckoff bond: `8c@4h`

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

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

Table 25: Wyckoff bond: `8a@8i`

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