SG No. 52 D_{2h}^{6} $Pnna$ [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	$[-X,\ Y,\ -Z]$	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[3,-7]`
4	$[X,\ -Y,\ -Z]$	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[4,-8]`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff bond: `8a@8e`

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