SG No. 51 D_{2h}^5 $Pmma$ [orthorhombic]

* plus set: $+[0, 0, 0]$

* Wyckoff site: 2a, site symmetry: .2/m.

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 2b@2a

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

Table 3: Wyckoff bond: 4c@2a

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

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

Table 4: Wyckoff bond: 2a@2b

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

Table 5: Wyckoff bond: 2b@2b

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

Table 6: Wyckoff bond: 4c@2b

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

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

Table 7: Wyckoff bond: 2a@2c

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

Table 8: Wyckoff bond: 2b@2c

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

Table 9: Wyckoff bond: 4c@2c

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	$[-X, Y, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	[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	$[X, 0, Z]$	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[1,-3,-5,7]
2	$[-X, 0, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[2,-4,-6,8]

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

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

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

Table 13: Wyckoff bond: `2a@2e`

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

Table 14: Wyckoff bond: `2b@2e`

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

Table 15: Wyckoff bond: `2c@2e`

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

Table 16: Wyckoff bond: 4d@2e

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

Table 17: Wyckoff bond: 4e@2e

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

Table 18: Wyckoff bond: 4f@2e

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

Table 19: Wyckoff bond: 8g@2e

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	$[-X, Y, -Z]$	$\left[\frac{3}{4}, 0, -z\right]$	[3]
4	$[X, -Y, -Z]$	$\left[\frac{3}{4}, 0, -z\right]$	[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	$[X, -Y, Z]$	$\left[\frac{1}{4}, 0, z\right]$	[7]
8	$[-X, Y, Z]$	$\left[\frac{1}{4}, 0, z\right]$	[8]

* Wyckoff site: 2f, site symmetry: mm2

Table 20: Wyckoff bond: `2a@2f`

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

Table 21: Wyckoff bond: `2b@2f`

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

Table 22: Wyckoff bond: `2c@2f`

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

Table 23: Wyckoff bond: `4d@2f`

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

Table 24: Wyckoff bond: `4e@2f`

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

Table 25: Wyckoff bond: `4f@2f`

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

Table 26: Wyckoff bond: `8g@2f`

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

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

Table 27: Wyckoff bond: `4a@4g`

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

Table 28: Wyckoff bond: `4b@4g`

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

Table 29: Wyckoff bond: 8c@4g

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

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

Table 30: Wyckoff bond: 4a@4h

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

Table 31: Wyckoff bond: 4b@4h

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

Table 32: Wyckoff bond: 8c@4h

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

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

Table 33: Wyckoff bond: `4a@4i`

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

Table 34: Wyckoff bond: `4b@4i`

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

Table 35: Wyckoff bond: `8c@4i`

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

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

Table 36: Wyckoff bond: `4a@4j`

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

Table 37: Wyckoff bond: `4b@4j`

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

Table 38: Wyckoff bond: `8c@4j`

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

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

Table 39: Wyckoff bond: `4a@4k`

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

Table 40: Wyckoff bond: `4b@4k`

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

Table 41: Wyckoff bond: `8c@4k`

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

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

Table 42: Wyckoff bond: `8a@8l`

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