SG No. 68 D_{2h}^{22} $Ccce$ [orthorhombic]

* plus set: $+[0, 0, 0]$, $+\left[\frac{1}{2}, \frac{1}{2}, 0\right]$
* Wyckoff site: 4a, site symmetry: 222

Table 1: Wyckoff bond: 4a@4a

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

Table 2: Wyckoff bond: 4b@4a

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

Table 3: Wyckoff bond: 4c@4a

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

Table 4: Wyckoff bond: 8d@4a

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

Table 5: Wyckoff bond: 8e@4a

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

Table 6: Wyckoff bond: `8f@4a`

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

Table 7: Wyckoff bond: `16g@4a`

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

* Wyckoff site: `4b`, site symmetry: `222`

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

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

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

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

Table 10: Wyckoff bond: `4c@4b`

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

Table 11: Wyckoff bond: `8d@4b`

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

Table 12: Wyckoff bond: `8e@4b`

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

Table 13: Wyckoff bond: `8f@4b`

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

Table 14: Wyckoff bond: `16g@4b`

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

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

Table 15: Wyckoff bond: 8a@8c

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

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

Table 16: Wyckoff bond: 8a@8d

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

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

Table 17: Wyckoff bond: 8a@8e

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 18: Wyckoff bond: 8b@8e

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 19: Wyckoff bond: 16c@8e

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]

continued ...

Table 19

No.	vector	center	mapping
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: 8f, site symmetry: .2.

Table 20: Wyckoff bond: 8a@8f

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

Table 21: Wyckoff bond: 8b@8f

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

Table 22: Wyckoff bond: 16c@8f

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

* Wyckoff site: 8g, site symmetry: ..2

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

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

Table 24: Wyckoff bond: `8b@8g`

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

Table 25: Wyckoff bond: `16c@8g`

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

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

Table 26: Wyckoff bond: `8a@8h`

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

Table 27: Wyckoff bond: `8b@8h`

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

Table 28: Wyckoff bond: `16c@8h`

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

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

Table 29: Wyckoff bond: `16a@16i`

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