SG No. 67 D_{2h}^{21} $Cmme$ [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	$[0,\ 0,\ Z]$	$\left[\frac{1}{4},\ 0,\ 0\right]$	`[1,2,-3,-4]`
2	$[0,\ 0,\ -Z]$	$\left[\frac{3}{4},\ 0,\ 0\right]$	`[5,6,-7,-8]`

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

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

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

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

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

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

Table 5: Wyckoff bond: `8e@4a`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 15: Wyckoff bond: `4a@4c`

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

Table 16: Wyckoff bond: `4b@4c`

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

Table 17: Wyckoff bond: `8c@4c`

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

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

Table 18: Wyckoff bond: `4a@4d`

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

Table 19: Wyckoff bond: `4b@4d`

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

Table 20: Wyckoff bond: `8c@4d`

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

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

Table 21: Wyckoff bond: `4a@4e`

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

Table 22: Wyckoff bond: `4b@4e`

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

Table 23: Wyckoff bond: `8c@4e`

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

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

Table 24: Wyckoff bond: `4a@4f`

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

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

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

Table 26: Wyckoff bond: `8c@4f`

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

* Wyckoff site: `4g`, site symmetry: `mm2`

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

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

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

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

Table 29: Wyckoff bond: `4c@4g`

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

Table 30: Wyckoff bond: `8d@4g`

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

Table 31: Wyckoff bond: `8e@4g`

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

Table 32: Wyckoff bond: `8f@4g`

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

Table 33: Wyckoff bond: `16g@4g`

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

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

Table 34: Wyckoff bond: `8a@8h`

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

Table 35: Wyckoff bond: `8b@8h`

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

Table 36: Wyckoff bond: `16c@8h`

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

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

Table 37: Wyckoff bond: `8a@8i`

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

Table 38: Wyckoff bond: `8b@8i`

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

Table 39: Wyckoff bond: `16c@8i`

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

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

Table 40: Wyckoff bond: `8a@8j`

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

Table 41: Wyckoff bond: `8b@8j`

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

Table 42: Wyckoff bond: `16c@8j`

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

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

Table 43: Wyckoff bond: `8a@8k`

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

Table 44: Wyckoff bond: `8b@8k`

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

Table 45: Wyckoff bond: `16c@8k`

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

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

Table 46: Wyckoff bond: 8a@8l

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

Table 47: Wyckoff bond: 8b@8l

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

Table 48: Wyckoff bond: 16c@8l

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	$[-X, Y, -Z]$	$\left[\frac{3}{4}, \frac{1}{2}, -z\right]$	[3]
4	$[X, -Y, -Z]$	$\left[\frac{3}{4}, \frac{1}{2}, -z\right]$	[4]
5	$[-X, -Y, -Z]$	$\left[\frac{3}{4}, 0, -z\right]$	[5]
6	$[X, Y, -Z]$	$\left[\frac{3}{4}, 0, -z\right]$	[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: 8m, site symmetry: m..

Table 49: Wyckoff bond: 8a@8m

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, z]$	[1,8]
2	$[0, -Y, Z]$	$\left[0, \frac{1}{2} - y, z\right]$	[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 50: Wyckoff bond: `8b@8m`

No.	vector	center	mapping
1	$[X,\ 0,\ 0]$	$[0,\ y,\ z]$	`[1,-8]`
2	$[-X,\ 0,\ 0]$	$\left[0,\ \frac{1}{2}-y,\ z\right]$	`[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 51: Wyckoff bond: `16c@8m`

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

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

Table 52: Wyckoff bond: `8a@8n`

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

Table 53: Wyckoff bond: `8b@8n`

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

Table 54: Wyckoff bond: `16c@8n`

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

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

Table 55: Wyckoff bond: `16a@16o`

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