SG No. 69 D_{2h}^{23} $Fmmm$ [orthorhombic]

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

Table 1: Wyckoff bond: `4a@4a`

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

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

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

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

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

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

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

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

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

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

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

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

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	`[1,-5]`
2	$[-X, -Y, Z]$	$[0, 0, 0]$	`[2,-6]`
3	$[-X, Y, -Z]$	$[0, 0, 0]$	`[3,-7]`
4	$[X, -Y, -Z]$	$[0, 0, 0]$	`[4,-8]`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

* Wyckoff site: `8c`, site symmetry: `2/m..`

Table 15: Wyckoff bond: `8a@8c`

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

Table 16: Wyckoff bond: `8b@8c`

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

Table 17: Wyckoff bond: `16c@8c`

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

* Wyckoff site: `8d`, site symmetry: `.2/m.`

Table 18: Wyckoff bond: `8a@8d`

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

Table 19: Wyckoff bond: `8b@8d`

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

Table 20: Wyckoff bond: `16c@8d`

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

* Wyckoff site: `8e`, site symmetry: `..2/m`

Table 21: Wyckoff bond: `8a@8e`

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

Table 22: Wyckoff bond: `8b@8e`

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

Table 23: Wyckoff bond: `16c@8e`

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

* Wyckoff site: `8f`, site symmetry: `222`

Table 24: Wyckoff bond: `8a@8f`

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

Table 25: Wyckoff bond: `8b@8f`

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

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

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

Table 27: Wyckoff bond: `16d@8f`

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

Table 28: Wyckoff bond: `16e@8f`

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

Table 29: Wyckoff bond: `16f@8f`

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

Table 30: Wyckoff bond: `32g@8f`

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

* Wyckoff site: `8g`, site symmetry: `2mm`

Table 31: Wyckoff bond: `8a@8g`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, 0, 0]$	`[1,-4,-6,7]`
2	$[0, 0, Z]$	$[-x, 0, 0]$	`[2,-3,-5,8]`

Table 32: Wyckoff bond: `8b@8g`

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, 0, 0]$	`[1,-4,6,-7]`

continued ...

Table 32

No.	vector	center	mapping
2	$[0, -Y, 0]$	$[-x, 0, 0]$	`[2,-3,5,-8]`

Table 33: Wyckoff bond: `8c@8g`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	`[1,4,6,7]`
2	$[-X, 0, 0]$	$[-x, 0, 0]$	`[2,3,5,8]`

Table 34: Wyckoff bond: `16d@8g`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, 0, 0]$	`[1,6]`
2	$[-X, -Y, 0]$	$[-x, 0, 0]$	`[2,5]`
3	$[-X, Y, 0]$	$[-x, 0, 0]$	`[3,8]`
4	$[X, -Y, 0]$	$[x, 0, 0]$	`[4,7]`

Table 35: Wyckoff bond: `16e@8g`

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, 0]$	`[1,7]`
2	$[-X, 0, Z]$	$[-x, 0, 0]$	`[2,8]`
3	$[-X, 0, -Z]$	$[-x, 0, 0]$	`[3,5]`
4	$[X, 0, -Z]$	$[x, 0, 0]$	`[4,6]`

Table 36: Wyckoff bond: `16f@8g`

No.	vector	center	mapping
1	$[0, Y, Z]$	$[x, 0, 0]$	`[1,-4]`
2	$[0, -Y, Z]$	$[-x, 0, 0]$	`[2,-3]`
3	$[0, -Y, -Z]$	$[-x, 0, 0]$	`[5,-8]`
4	$[0, Y, -Z]$	$[x, 0, 0]$	`[6,-7]`

Table 37: Wyckoff bond: `32g@8g`

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

* Wyckoff site: `8h`, site symmetry: `m2m`

Table 38: Wyckoff bond: `8a@8h`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, y, 0]$	`[1,-3,-6,8]`
2	$[0, 0, Z]$	$[0, -y, 0]$	`[2,-4,-5,7]`

Table 39: Wyckoff bond: `8b@8h`

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, y, 0]$	`[1,3,6,8]`
2	$[0, -Y, 0]$	$[0, -y, 0]$	`[2,4,5,7]`

Table 40: Wyckoff bond: `8c@8h`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, 0]$	`[1,-3,6,-8]`
2	$[-X, 0, 0]$	$[0, -y, 0]$	`[2,-4,5,-7]`

Table 41: Wyckoff bond: `16d@8h`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, y, 0]$	`[1,6]`
2	$[-X, -Y, 0]$	$[0, -y, 0]$	`[2,5]`
3	$[-X, Y, 0]$	$[0, y, 0]$	`[3,8]`
4	$[X, -Y, 0]$	$[0, -y, 0]$	`[4,7]`

Table 42: Wyckoff bond: `16e@8h`

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, y, 0]$	`[1,-3]`
2	$[-X, 0, Z]$	$[0, -y, 0]$	`[2,-4]`
3	$[-X, 0, -Z]$	$[0, -y, 0]$	`[5,-7]`
4	$[X, 0, -Z]$	$[0, y, 0]$	`[6,-8]`

Table 43: Wyckoff bond: `16f@8h`

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, 0]$	`[1,8]`
2	$[0, -Y, Z]$	$[0, -y, 0]$	`[2,7]`
3	$[0, Y, -Z]$	$[0, y, 0]$	`[3,6]`
4	$[0, -Y, -Z]$	$[0, -y, 0]$	`[4,5]`

Table 44: Wyckoff bond: `32g@8h`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, 0]$	`[1]`
2	$[-X, -Y, Z]$	$[0, -y, 0]$	`[2]`
3	$[-X, Y, -Z]$	$[0, y, 0]$	`[3]`
4	$[X, -Y, -Z]$	$[0, -y, 0]$	`[4]`
5	$[-X, -Y, -Z]$	$[0, -y, 0]$	`[5]`
6	$[X, Y, -Z]$	$[0, y, 0]$	`[6]`
7	$[X, -Y, Z]$	$[0, -y, 0]$	`[7]`
8	$[-X, Y, Z]$	$[0, y, 0]$	`[8]`

* Wyckoff site: `8i`, site symmetry: `mm2`

Table 45: Wyckoff bond: `8a@8i`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	`[1,2,7,8]`
2	$[0, 0, -Z]$	$[0, 0, -z]$	`[3,4,5,6]`

Table 46: Wyckoff bond: `8b@8i`

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, 0, z]$	`[1,-2,-7,8]`

continued ...

Table 46

No.	vector	center	mapping
2	[0, Y, 0]	[0, 0, $-z$]	`[3,-4,-5,6]`

Table 47: Wyckoff bond: `8c@8i`

No.	vector	center	mapping
1	[X, 0, 0]	[0, 0, z]	`[1,-2,7,-8]`
2	[$-X$, 0, 0]	[0, 0, $-z$]	`[3,-4,5,-6]`

Table 48: Wyckoff bond: `16d@8i`

No.	vector	center	mapping
1	[X, Y, 0]	[0, 0, z]	`[1,-2]`
2	[$-X$, Y, 0]	[0, 0, $-z$]	`[3,-4]`
3	[$-X$, $-Y$, 0]	[0, 0, $-z$]	`[5,-6]`
4	[X, $-Y$, 0]	[0, 0, z]	`[7,-8]`

Table 49: Wyckoff bond: `16e@8i`

No.	vector	center	mapping
1	[X, 0, Z]	[0, 0, z]	`[1,7]`
2	[$-X$, 0, Z]	[0, 0, z]	`[2,8]`
3	[$-X$, 0, $-Z$]	[0, 0, $-z$]	`[3,5]`
4	[X, 0, $-Z$]	[0, 0, $-z$]	`[4,6]`

Table 50: Wyckoff bond: `16f@8i`

No.	vector	center	mapping
1	[0, Y, Z]	[0, 0, z]	`[1,8]`
2	[0, $-Y$, Z]	[0, 0, z]	`[2,7]`
3	[0, Y, $-Z$]	[0, 0, $-z$]	`[3,6]`
4	[0, $-Y$, $-Z$]	[0, 0, $-z$]	`[4,5]`

Table 51: Wyckoff bond: `32g@8i`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	`[1]`
2	$[-X, -Y, Z]$	$[0, 0, z]$	`[2]`
3	$[-X, Y, -Z]$	$[0, 0, -z]$	`[3]`
4	$[X, -Y, -Z]$	$[0, 0, -z]$	`[4]`
5	$[-X, -Y, -Z]$	$[0, 0, -z]$	`[5]`
6	$[X, Y, -Z]$	$[0, 0, -z]$	`[6]`
7	$[X, -Y, Z]$	$[0, 0, z]$	`[7]`
8	$[-X, Y, Z]$	$[0, 0, z]$	`[8]`

* Wyckoff site: `16j`, site symmetry: `..2`

Table 52: Wyckoff bond: `16a@16j`

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

Table 53: Wyckoff bond: `16b@16j`

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

Table 54: Wyckoff bond: `32c@16j`

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

* Wyckoff site: `16k`, site symmetry: `.2.`

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

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

Table 56: Wyckoff bond: `16b@16k`

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

Table 57: Wyckoff bond: `32c@16k`

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

* Wyckoff site: `16l`, site symmetry: `2..`

Table 58: Wyckoff bond: `16a@16l`

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

Table 59: Wyckoff bond: `16b@16l`

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

Table 60: Wyckoff bond: `32c@16l`

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

* Wyckoff site: `16m`, site symmetry: `m..`

Table 61: Wyckoff bond: `16a@16m`

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

Table 62: Wyckoff bond: `16b@16m`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	`[1,-8]`
2	$[-X, 0, 0]$	$[0, -y, z]$	`[2,-7]`
3	$[-X, 0, 0]$	$[0, y, -z]$	`[3,-6]`
4	$[X, 0, 0]$	$[0, -y, -z]$	`[4,-5]`

Table 63: Wyckoff bond: `32c@16m`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, z]$	`[1]`
2	$[-X, -Y, Z]$	$[0, -y, z]$	`[2]`
3	$[-X, Y, -Z]$	$[0, y, -z]$	`[3]`
4	$[X, -Y, -Z]$	$[0, -y, -z]$	`[4]`
5	$[-X, -Y, -Z]$	$[0, -y, -z]$	`[5]`
6	$[X, Y, -Z]$	$[0, y, -z]$	`[6]`
7	$[X, -Y, Z]$	$[0, -y, z]$	`[7]`
8	$[-X, Y, Z]$	$[0, y, z]$	`[8]`

* Wyckoff site: `16n`, site symmetry: `.m.`

Table 64: Wyckoff bond: `16a@16n`

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

Table 65: Wyckoff bond: `16b@16n`

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, 0, z]$	`[1,-7]`
2	$[0, -Y, 0]$	$[-x, 0, z]$	`[2,-8]`
3	$[0, Y, 0]$	$[-x, 0, -z]$	`[3,-5]`
4	$[0, -Y, 0]$	$[x, 0, -z]$	`[4,-6]`

Table 66: Wyckoff bond: `32c@16n`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, z]$	`[1]`
2	$[-X, -Y, Z]$	$[-x, 0, z]$	`[2]`
3	$[-X, Y, -Z]$	$[-x, 0, -z]$	`[3]`
4	$[X, -Y, -Z]$	$[x, 0, -z]$	`[4]`
5	$[-X, -Y, -Z]$	$[-x, 0, -z]$	`[5]`
6	$[X, Y, -Z]$	$[x, 0, -z]$	`[6]`
7	$[X, -Y, Z]$	$[x, 0, z]$	`[7]`
8	$[-X, Y, Z]$	$[-x, 0, z]$	`[8]`

* Wyckoff site: 16o, site symmetry: ..m

Table 67: Wyckoff bond: 16a@16o

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, y, 0]$	[1,6]
2	$[-X, -Y, 0]$	$[-x, -y, 0]$	[2,5]
3	$[-X, Y, 0]$	$[-x, y, 0]$	[3,8]
4	$[X, -Y, 0]$	$[x, -y, 0]$	[4,7]

Table 68: Wyckoff bond: 16b@16o

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, y, 0]$	[1,-6]
2	$[0, 0, Z]$	$[-x, -y, 0]$	[2,-5]
3	$[0, 0, -Z]$	$[-x, y, 0]$	[3,-8]
4	$[0, 0, -Z]$	$[x, -y, 0]$	[4,-7]

Table 69: Wyckoff bond: 32c@16o

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, 0]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, 0]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, 0]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, 0]$	[4]
5	$[-X, -Y, -Z]$	$[-x, -y, 0]$	[5]
6	$[X, Y, -Z]$	$[x, y, 0]$	[6]
7	$[X, -Y, Z]$	$[x, -y, 0]$	[7]
8	$[-X, Y, Z]$	$[-x, y, 0]$	[8]

* Wyckoff site: 32p, site symmetry: 1

Table 70: Wyckoff bond: 32a@32p

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, -z]$	[4]
5	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[5]
6	$[X, Y, -Z]$	$[x, y, -z]$	[6]
7	$[X, -Y, Z]$	$[x, -y, z]$	[7]

8	$[-X, Y, Z]$	$[-x, y, z]$	[8]