SG No. 65 D_{2h}^{19} $Cmmm$ [orthorhombic]

* plus set: $+[0, 0, 0], \quad +\left[\frac{1}{2}, \frac{1}{2}, 0\right]$

* Wyckoff site: 2a, site symmetry: mmm

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 2b@2a

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

Table 3: Wyckoff bond: 2c@2a

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

Table 4: Wyckoff bond: 4d@2a

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: 4e@2a

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: 4f@2a

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: 8g@2a

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: 2b, site symmetry: mmm

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 2b@2b

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

Table 10: Wyckoff bond: 2c@2b

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

Table 11: Wyckoff bond: 4d@2b

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

Table 12: Wyckoff bond: 4e@2b

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

Table 13: Wyckoff bond: 4f@2b

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

Table 14: Wyckoff bond: 8g@2b

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

* Wyckoff site: 2c, site symmetry: mmm

Table 15: Wyckoff bond: 2a@2c

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

Table 16: Wyckoff bond: 2b@2c

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

Table 17: Wyckoff bond: 2c@2c

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

Table 18: Wyckoff bond: 4d@2c

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

3

Table 19: Wyckoff bond: 4e@2c

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

Table 20: Wyckoff bond: 4f@2c

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

Table 21: Wyckoff bond: 8g@2c

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

* Wyckoff site: 2d, site symmetry: mmm

Table 22: Wyckoff bond: 2a@2d

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

Table 23: Wyckoff bond: 2b@2d

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

Table 24: Wyckoff bond: 2c@2d

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

Table 25: Wyckoff bond: 4d@2d

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 26: Wyckoff bond: 4e@2d

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 27: Wyckoff bond: 4f@2d

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 28: Wyckoff bond: 8g@2d

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: 4e, site symmetry: ..2/m

Table 29: Wyckoff bond: 4a@4e

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]

5

Table 30: Wyckoff bond: 4b@4e

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 31: Wyckoff bond: 8c@4e

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[1,-5]
2	$[-X, -Y, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[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: 4f, site symmetry: ..2/m

Table 32: Wyckoff bond: 4a@4f

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

Table 33: Wyckoff bond: 4b@4f

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

Table 34: 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	$[-X, -Y, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[2,-6]
3	$[-X, Y, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[3,-7]
4	$[X, -Y, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[4,-8]

* Wyckoff site: 4g, site symmetry: 2mm

Table 35: Wyckoff bond: `4a@4g`

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 36: Wyckoff bond: `4b@4g`

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

Table 37: Wyckoff bond: `4c@4g`

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 38: Wyckoff bond: `8d@4g`

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 39: Wyckoff bond: `8e@4g`

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 40: Wyckoff bond: 8f@4g

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 41: Wyckoff bond: 16g@4g

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: 4h, site symmetry: 2mm

Table 42: Wyckoff bond: 4a@4h

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

Table 43: Wyckoff bond: 4b@4h

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

Table 44: Wyckoff bond: 4c@4h

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

Table 45: Wyckoff bond: `8d@4h`

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

Table 46: Wyckoff bond: `8e@4h`

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

Table 47: Wyckoff bond: `8f@4h`

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

Table 48: Wyckoff bond: `16g@4h`

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

* Wyckoff site: `4i`, site symmetry: `m2m`

Table 49: Wyckoff bond: `4a@4i`

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 50: Wyckoff bond: `4b@4i`

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 51: Wyckoff bond: `4c@4i`

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 52: Wyckoff bond: `8d@4i`

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 53: Wyckoff bond: `8e@4i`

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 54: Wyckoff bond: `8f@4i`

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 55: Wyckoff bond: `16g@4i`

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: `4j`, site symmetry: `m2m`

Table 56: Wyckoff bond: `4a@4j`

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

Table 57: Wyckoff bond: `4b@4j`

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

Table 58: Wyckoff bond: `4c@4j`

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

Table 59: Wyckoff bond: `8d@4j`

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

Table 60: Wyckoff bond: `8e@4j`

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

Table 61: Wyckoff bond: `8f@4j`

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

Table 62: Wyckoff bond: `16g@4j`

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

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

Table 63: Wyckoff bond: 4a@4k

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 64: Wyckoff bond: 4b@4k

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

Table 65: Wyckoff bond: 4c@4k

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 66: Wyckoff bond: 8d@4k

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 67: Wyckoff bond: 8e@4k

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 68: Wyckoff bond: `8f@4k`

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 69: Wyckoff bond: `16g@4k`

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: `4l`, site symmetry: `mm2`

Table 70: Wyckoff bond: `4a@4l`

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

Table 71: Wyckoff bond: `4b@4l`

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

Table 72: Wyckoff bond: `4c@4l`

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

Table 73: Wyckoff bond: `8d@4l`

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

Table 74: Wyckoff bond: `8e@4l`

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

Table 75: Wyckoff bond: `8f@4l`

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

Table 76: Wyckoff bond: `16g@4l`

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

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

Table 77: Wyckoff bond: `8a@8m`

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 78: Wyckoff bond: `8b@8m`

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 79: Wyckoff bond: `16c@8m`

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

Table 80: Wyckoff bond: `8a@8n`

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 81: Wyckoff bond: 8b@8n

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 82: Wyckoff bond: 16c@8n

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: 8o, site symmetry: .m.

Table 83: Wyckoff bond: 8a@8o

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 84: Wyckoff bond: 8b@8o

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 85: Wyckoff bond: `16c@8o`

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: `8p`, site symmetry: `..m`

Table 86: Wyckoff bond: `8a@8p`

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 87: Wyckoff bond: `8b@8p`

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 88: Wyckoff bond: `16c@8p`

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: 8q, site symmetry: ..m

Table 89: Wyckoff bond: 8a@8q

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

Table 90: Wyckoff bond: 8b@8q

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

Table 91: Wyckoff bond: 16c@8q

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

* Wyckoff site: 16r, site symmetry: 1

Table 92: Wyckoff bond: 16a@16r

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]

continued ...

Table 92

No.	vector	center	mapping
8	$[-X,\,Y,\,Z]$	$[-x,\,y,\,z]$	[8]