SG No. 16 D_2^1 $P222$ [orthorhombic]

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

* Wyckoff site: 1a, site symmetry: 222

Table 1: Wyckoff bond: 1a@1a

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

Table 2: Wyckoff bond: 1b@1a

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

Table 3: Wyckoff bond: 1c@1a

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

Table 4: Wyckoff bond: 2d@1a

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	[1,-2]
2	$[-X, Y, 0]$	$[0, 0, 0]$	[3,-4]

Table 5: Wyckoff bond: 2e@1a

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, 0]$	[1,-3]
2	$[-X, 0, Z]$	$[0, 0, 0]$	[2,-4]

Table 6: Wyckoff bond: 2f@1a

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, 0, 0]$	[1,-4]
2	$[0, -Y, Z]$	$[0, 0, 0]$	[2,-3]

Table 7: Wyckoff bond: `4g@1a`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	[1]
2	$[-X, -Y, Z]$	$[0, 0, 0]$	[2]
3	$[-X, Y, -Z]$	$[0, 0, 0]$	[3]
4	$[X, -Y, -Z]$	$[0, 0, 0]$	[4]

* Wyckoff site: `1b`, site symmetry: `222`

Table 8: Wyckoff bond: `1a@1b`

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

Table 9: Wyckoff bond: `1b@1b`

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

Table 10: Wyckoff bond: `1c@1b`

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

Table 11: Wyckoff bond: `2d@1b`

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

Table 12: Wyckoff bond: `2e@1b`

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

Table 13: Wyckoff bond: 2f@1b

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

Table 14: Wyckoff bond: 4g@1b

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

* Wyckoff site: 1c, site symmetry: 222

Table 15: Wyckoff bond: 1a@1c

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

Table 16: Wyckoff bond: 1b@1c

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

Table 17: Wyckoff bond: 1c@1c

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

Table 18: Wyckoff bond: 2d@1c

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

Table 19: Wyckoff bond: `2e@1c`

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

Table 20: Wyckoff bond: `2f@1c`

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

Table 21: Wyckoff bond: `4g@1c`

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

* Wyckoff site: `1d`, site symmetry: `222`

Table 22: Wyckoff bond: `1a@1d`

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

Table 23: Wyckoff bond: `1b@1d`

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

Table 24: Wyckoff bond: `1c@1d`

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

Table 25: Wyckoff bond: 2d@1d

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

Table 26: Wyckoff bond: 2e@1d

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

Table 27: Wyckoff bond: 2f@1d

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

Table 28: Wyckoff bond: 4g@1d

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

* Wyckoff site: 1e, site symmetry: 222

Table 29: Wyckoff bond: 1a@1e

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

Table 30: Wyckoff bond: 1b@1e

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

Table 31: Wyckoff bond: `1c@1e`

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

Table 32: Wyckoff bond: `2d@1e`

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

Table 33: Wyckoff bond: `2e@1e`

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

Table 34: Wyckoff bond: `2f@1e`

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

Table 35: Wyckoff bond: `4g@1e`

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

* Wyckoff site: `1f`, site symmetry: `222`

Table 36: Wyckoff bond: `1a@1f`

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

Table 37: Wyckoff bond: `1b@1f`

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

Table 38: Wyckoff bond: `1c@1f`

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

Table 39: Wyckoff bond: `2d@1f`

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

Table 40: Wyckoff bond: `2e@1f`

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

Table 41: Wyckoff bond: `2f@1f`

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

Table 42: Wyckoff bond: `4g@1f`

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

* Wyckoff site: `1g`, site symmetry: `222`

Table 43: Wyckoff bond: `1a@1g`

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

Table 44: Wyckoff bond: `1b@1g`

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

Table 45: Wyckoff bond: `1c@1g`

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

Table 46: Wyckoff bond: `2d@1g`

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

Table 47: Wyckoff bond: `2e@1g`

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

Table 48: Wyckoff bond: `2f@1g`

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

Table 49: Wyckoff bond: `4g@1g`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[1]
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[2]
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[3]
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[4]

* Wyckoff site: `1h`, site symmetry: `222`

Table 50: Wyckoff bond: `1a@1h`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1,2,-3,-4]

Table 51: Wyckoff bond: `1b@1h`

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1,-2,3,-4]

Table 52: Wyckoff bond: `1c@1h`

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1,-2,-3,4]

Table 53: Wyckoff bond: `2d@1h`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1,-2]
2	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[3,-4]

Table 54: Wyckoff bond: `2e@1h`

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1,-3]
2	$[-X, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[2,-4]

Table 55: Wyckoff bond: 2f@1h

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

Table 56: Wyckoff bond: 4g@1h

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

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

Table 57: Wyckoff bond: 2a@2i

No.	vector	center	mapping
1	$[0, Y, Z]$	$[x, 0, 0]$	[1,-4]
2	$[0, -Y, Z]$	$[-x, 0, 0]$	[2,-3]

Table 58: Wyckoff bond: 2b@2i

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	[1,4]
2	$[-X, 0, 0]$	$[-x, 0, 0]$	[2,3]

Table 59: Wyckoff bond: 4c@2i

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]

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

Table 60: Wyckoff bond: `2a@2j`

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]

Table 61: Wyckoff bond: `2b@2j`

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

Table 62: Wyckoff bond: `4c@2j`

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]

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

Table 63: Wyckoff bond: `2a@2k`

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

Table 64: Wyckoff bond: `2b@2k`

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

Table 65: Wyckoff bond: 4c@2k

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

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

Table 66: Wyckoff bond: 2a@2l

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

Table 67: Wyckoff bond: 2b@2l

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

Table 68: Wyckoff bond: 4c@2l

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

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

Table 69: Wyckoff bond: 2a@2m

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, y, 0]$	[1,-3]
2	$[-X, 0, Z]$	$[0, -y, 0]$	[2,-4]

Table 70: Wyckoff bond: 2b@2m

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, y, 0]$	[1,3]
2	$[0, -Y, 0]$	$[0, -y, 0]$	[2,4]

Table 71: Wyckoff bond: 4c@2m

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]

* Wyckoff site: 2n, site symmetry: .2.

Table 72: Wyckoff bond: 2a@2n

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]

Table 73: Wyckoff bond: 2b@2n

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

Table 74: Wyckoff bond: 4c@2n

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]

* Wyckoff site: 2o, site symmetry: .2.

Table 75: Wyckoff bond: 2a@2o

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

Table 76: Wyckoff bond: 2b@2o

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

Table 77: Wyckoff bond: 4c@2o

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

* Wyckoff site: 2p, site symmetry: .2.

Table 78: Wyckoff bond: 2a@2p

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

Table 79: Wyckoff bond: 2b@2p

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

Table 80: Wyckoff bond: `4c@2p`

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

* Wyckoff site: `2q`, site symmetry: `..2`

Table 81: Wyckoff bond: `2a@2q`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	[1,-2]
2	$[-X, Y, 0]$	$[0, 0, -z]$	[3,-4]

Table 82: Wyckoff bond: `2b@2q`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	[1,2]
2	$[0, 0, -Z]$	$[0, 0, -z]$	[3,4]

Table 83: Wyckoff bond: `4c@2q`

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]

* Wyckoff site: `2r`, site symmetry: `..2`

Table 84: Wyckoff bond: `2a@2r`

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

Table 85: Wyckoff bond: 2b@2r

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

Table 86: Wyckoff bond: 4c@2r

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

* Wyckoff site: 2s, site symmetry: ..2

Table 87: Wyckoff bond: 2a@2s

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]

Table 88: Wyckoff bond: 2b@2s

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

Table 89: Wyckoff bond: 4c@2s

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]

* Wyckoff site: 2t, site symmetry: ..2

Table 90: Wyckoff bond: `2a@2t`

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

Table 91: Wyckoff bond: `2b@2t`

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

Table 92: Wyckoff bond: `4c@2t`

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

* Wyckoff site: `4u`, site symmetry: `1`

Table 93: Wyckoff bond: `4a@4u`

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]