

SG No. 89 D_4^1 P422 [tetragonal]

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

* Wyckoff site: 1a, site symmetry: 422

Table 1: Wyckoff bond: 1a@1a

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

Table 2: Wyckoff bond: 2b@1a

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

Table 3: Wyckoff bond: 2c@1a

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

Table 4: Wyckoff bond: 4d@1a

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

Table 5: Wyckoff bond: 4e@1a

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

Table 6: Wyckoff bond: 4f@1a

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

Table 7: Wyckoff bond: 8g@1a

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

* Wyckoff site: 1b, site symmetry: 422

Table 8: Wyckoff bond: 1a@1b

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

Table 9: Wyckoff bond: 2b@1b

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

Table 10: Wyckoff bond: 2c@1b

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

Table 11: Wyckoff bond: 4d@1b

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

Table 12: Wyckoff bond: 4e@1b

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

Table 13: Wyckoff bond: 4f@1b

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

Table 14: Wyckoff bond: 8g@1b

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

* Wyckoff site: 1c, site symmetry: 422

Table 15: Wyckoff bond: 1a@1c

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

Table 16: Wyckoff bond: 2b@1c

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

Table 17: Wyckoff bond: 2c@1c

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

Table 18: Wyckoff bond: 4d@1c

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

Table 19: Wyckoff bond: 4e@1c

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

Table 20: Wyckoff bond: 4f@1c

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

continued ...

Table 20

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

Table 21: Wyckoff bond: 8g@1c

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

* Wyckoff site: 1d, site symmetry: 422

Table 22: Wyckoff bond: 1a@1d

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

Table 23: Wyckoff bond: 2b@1d

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

Table 24: Wyckoff bond: 2c@1d

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

Table 25: Wyckoff bond: 4d@1d

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

Table 26: Wyckoff bond: 4e@1d

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

Table 27: Wyckoff bond: 4f@1d

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

Table 28: Wyckoff bond: 8g@1d

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

* Wyckoff site: 2e, site symmetry: 222.

Table 29: Wyckoff bond: 2a@2e

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

Table 30: Wyckoff bond: 2b@2e

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

Table 31: Wyckoff bond: 2c@2e

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

Table 32: Wyckoff bond: 4d@2e

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

Table 33: Wyckoff bond: 4e@2e

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

Table 34: Wyckoff bond: 4f@2e

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

Table 35: Wyckoff bond: 8g@2e

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

* Wyckoff site: 2f, site symmetry: 222.

Table 36: Wyckoff bond: 2a@2f

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

Table 37: Wyckoff bond: 2b@2f

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

Table 38: Wyckoff bond: 2c@2f

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

Table 39: Wyckoff bond: 4d@2f

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

Table 40: Wyckoff bond: 4e@2f

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

Table 41: Wyckoff bond: 4f@2f

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

Table 42: Wyckoff bond: 8g@2f

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

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

Table 43: Wyckoff bond: 2a@2g

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

Table 44: Wyckoff bond: 4b@2g

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

Table 45: Wyckoff bond: 8c@2g

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

* Wyckoff site: 2h, site symmetry: 4..

Table 46: Wyckoff bond: 2a@2h

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

Table 47: Wyckoff bond: 4b@2h

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

continued ...

Table 47

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

Table 48: Wyckoff bond: 8c@2h

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

* Wyckoff site: 4i, site symmetry: 2..

Table 49: Wyckoff bond: 4a@4i

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

Table 50: Wyckoff bond: 4b@4i

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

Table 51: Wyckoff bond: 8c@4i

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

continued ...

Table 51

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

* Wyckoff site: 4j, site symmetry: . . 2

Table 52: Wyckoff bond: 4a@4j

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

Table 53: Wyckoff bond: 4b@4j

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

Table 54: Wyckoff bond: 8c@4j

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

* Wyckoff site: 4k, site symmetry: . . 2

Table 55: Wyckoff bond: 4a@4k

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

Table 56: Wyckoff bond: 4b@4k

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

Table 57: Wyckoff bond: 8c@4k

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

* Wyckoff site: 41, site symmetry: .2.

Table 58: Wyckoff bond: 4a@41

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

Table 59: Wyckoff bond: 4b@4l

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

Table 60: Wyckoff bond: 8c@4l

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

* Wyckoff site: 4m, site symmetry: .2.

Table 61: Wyckoff bond: 4a@4m

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

Table 62: Wyckoff bond: 4b@4m

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

Table 63: Wyckoff bond: 8c@4m

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

* Wyckoff site: 4n, site symmetry: .2.

Table 64: Wyckoff bond: 4a@4n

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

Table 65: Wyckoff bond: 4b@4n

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

Table 66: Wyckoff bond: 8c@4n

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

* Wyckoff site: 4o, site symmetry: .2.

Table 67: Wyckoff bond: 4a@4o

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

Table 68: Wyckoff bond: 4b@4o

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

Table 69: Wyckoff bond: 8c@4o

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

* Wyckoff site: 8p, site symmetry: 1

Table 70: Wyckoff bond: 8a@8p

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

$$\begin{array}{cccc} \hline & 8 & [-Y, -X, -Z] & [-y, -x, -z] \\ \hline \hline & [8] & & \end{array}$$