

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:  $\dots 2$

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:  $\dots 2$

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: **4l**, site symmetry:  $.2$ .

Table 58: Wyckoff bond: **4a@4l**

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@41**

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@41**

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	$[Y, X, -Z]$	$[y, x, -z]$	$[7]$

