

SG No. 136  $D_{4h}^{14}$   $P4_2/mnm$  [ tetragonal ]

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

\* Wyckoff site: 2a, site symmetry: m.mmm

Table 1: Wyckoff bond: 2a@2a

No.	vector	center	mapping
1	$[X, X, 0]$	$[0, 0, 0]$	$[1, -2, 7, -8, -9, 10, -15, 16]$
2	$[-X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, -4, 5, -6, -11, 12, -13, 14]$

Table 2: Wyckoff bond: 2b@2a

No.	vector	center	mapping
1	$[X, -X, 0]$	$[0, 0, 0]$	$[1, -2, -7, 8, -9, 10, 15, -16]$
2	$[X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, -4, -5, 6, -11, 12, 13, -14]$

Table 3: Wyckoff bond: 2c@2a

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	$[1, 2, -7, -8, -9, -10, 15, 16]$
2	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, 4, -5, -6, -11, -12, 13, 14]$

Table 4: Wyckoff bond: 4d@2a

No.	vector	center	mapping
1	$[X, X, Z]$	$[0, 0, 0]$	$[1, -8, -9, 16]$
2	$[-X, -X, Z]$	$[0, 0, 0]$	$[2, -7, -10, 15]$
3	$[-X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, -6, -11, 14]$
4	$[X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[4, -5, -12, 13]$

Table 5: Wyckoff bond: 4e@2a

No.	vector	center	mapping
1	$[X, -X, Z]$	$[0, 0, 0]$	$[1, -7, -9, 15]$
2	$[-X, X, Z]$	$[0, 0, 0]$	$[2, -8, -10, 16]$
3	$[X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, -5, -11, 13]$
4	$[-X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[4, -6, -12, 14]$

Table 6: Wyckoff bond: 4f@2a

No.	vector	center	mapping
1	[X, Y, 0]	[0, 0, 0]	[1, -2, -9, 10]
2	[-Y, X, 0]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[3, -4, -11, 12]
3	[-X, Y, 0]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[5, -6, -13, 14]
4	[Y, X, 0]	[0, 0, 0]	[7, -8, -15, 16]

Table 7: Wyckoff bond: 8g@2a

No.	vector	center	mapping
1	[X, Y, Z]	[0, 0, 0]	[1, -9]
2	[-X, -Y, Z]	[0, 0, 0]	[2, -10]
3	[-Y, X, Z]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[3, -11]
4	[Y, -X, Z]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[4, -12]
5	[-X, Y, -Z]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[5, -13]
6	[X, -Y, -Z]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[6, -14]
7	[Y, X, -Z]	[0, 0, 0]	[7, -15]
8	[-Y, -X, -Z]	[0, 0, 0]	[8, -16]

\* Wyckoff site: 2b, site symmetry: **m.m̄m**

Table 8: Wyckoff bond: 2a@2b

No.	vector	center	mapping
1	[X, X, 0]	[0, 0, \frac{1}{2}]	[1, -2, 7, -8, -9, 10, -15, 16]
2	[-X, X, 0]	[\frac{1}{2}, \frac{1}{2}, 0]	[3, -4, 5, -6, -11, 12, -13, 14]

Table 9: Wyckoff bond: 2b@2b

No.	vector	center	mapping
1	[X, -X, 0]	[0, 0, \frac{1}{2}]	[1, -2, -7, 8, -9, 10, 15, -16]
2	[X, X, 0]	[\frac{1}{2}, \frac{1}{2}, 0]	[3, -4, -5, 6, -11, 12, 13, -14]

Table 10: Wyckoff bond: 2c@2b

No.	vector	center	mapping
1	[0, 0, Z]	[0, 0, \frac{1}{2}]	[1, 2, -7, -8, -9, -10, 15, 16]
2	[0, 0, Z]	[\frac{1}{2}, \frac{1}{2}, 0]	[3, 4, -5, -6, -11, -12, 13, 14]

Table 11: Wyckoff bond: 4d@2b

No.	vector	center	mapping
1	$[X, X, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -8, -9, 16]$
2	$[-X, -X, Z]$	$[0, 0, \frac{1}{2}]$	$[2, -7, -10, 15]$
3	$[-X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[3, -6, -11, 14]$
4	$[X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[4, -5, -12, 13]$

Table 12: Wyckoff bond: 4e@2b

No.	vector	center	mapping
1	$[X, -X, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -7, -9, 15]$
2	$[-X, X, Z]$	$[0, 0, \frac{1}{2}]$	$[2, -8, -10, 16]$
3	$[X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[3, -5, -11, 13]$
4	$[-X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[4, -6, -12, 14]$

Table 13: Wyckoff bond: 4f@2b

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, \frac{1}{2}]$	$[1, -2, -9, 10]$
2	$[-Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[3, -4, -11, 12]$
3	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[5, -6, -13, 14]$
4	$[Y, X, 0]$	$[0, 0, \frac{1}{2}]$	$[7, -8, -15, 16]$

Table 14: Wyckoff bond: 8g@2b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -9]$
2	$[-X, -Y, Z]$	$[0, 0, \frac{1}{2}]$	$[2, -10]$
3	$[-Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[3, -11]$
4	$[Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[4, -12]$
5	$[-X, Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[5, -13]$
6	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[6, -14]$
7	$[Y, X, -Z]$	$[0, 0, \frac{1}{2}]$	$[7, -15]$
8	$[-Y, -X, -Z]$	$[0, 0, \frac{1}{2}]$	$[8, -16]$

\* Wyckoff site: 4c, site symmetry: 2/m..

Table 15: Wyckoff bond: 4a@4c

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, 0]$	$[1, -2, -9, 10]$
2	$[-Y, X, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -4, -11, 12]$
3	$[-X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6, -13, 14]$
4	$[Y, X, 0]$	$[\frac{1}{2}, 0, 0]$	$[7, -8, -15, 16]$

Table 16: Wyckoff bond: 4b@4c

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, 0]$	$[1, 2, -9, -10]$
2	$[0, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, 4, -11, -12]$
3	$[0, 0, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, 6, -13, -14]$
4	$[0, 0, -Z]$	$[\frac{1}{2}, 0, 0]$	$[7, 8, -15, -16]$

Table 17: Wyckoff bond: 8c@4c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, 0]$	$[1, -9]$
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, 0]$	$[2, -10]$
3	$[-Y, X, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -11]$
4	$[Y, -X, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[4, -12]$
5	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -13]$
6	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, -14]$
7	$[Y, X, -Z]$	$[\frac{1}{2}, 0, 0]$	$[7, -15]$
8	$[-Y, -X, -Z]$	$[\frac{1}{2}, 0, 0]$	$[8, -16]$

\* Wyckoff site: 4d, site symmetry: -4..

Table 18: Wyckoff bond: 4a@4d

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, 2, -11, -12]$
2	$[0, 0, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[3, 4, -9, -10]$
3	$[0, 0, -Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[5, 6, -15, -16]$
4	$[0, 0, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[7, 8, -13, -14]$

Table 19: Wyckoff bond: 8b@4d

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[1,-2]
2	$[-Y, X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[3,-4]
3	$[-X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[5,-6]
4	$[Y, X, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[7,-8]
5	$[-X, -Y, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[9,-10]
6	$[Y, -X, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[11,-12]
7	$[X, -Y, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[13,-14]
8	$[-Y, -X, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[15,-16]

Table 20: Wyckoff bond: 16c@4d

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[1]
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[2]
3	$[-Y, X, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[3]
4	$[Y, -X, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[4]
5	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[5]
6	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[6]
7	$[Y, X, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[7]
8	$[-Y, -X, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[8]
9	$[-X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[9]
10	$[X, Y, -Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[10]
11	$[Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[11]
12	$[-Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[12]
13	$[X, -Y, Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[14]
15	$[-Y, -X, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[15]
16	$[Y, X, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[16]

\* Wyckoff site: 4e, site symmetry: 2.mm

Table 21: Wyckoff bond: 4a@4e

No.	vector	center	mapping
1	$[X, X, 0]$	$[0, 0, z]$	[1,-2,-15,16]
2	$[-X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[3,-4,-13,14]
3	$[-X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[5,-6,-11,12]
4	$[X, X, 0]$	$[0, 0, -z]$	[7,-8,-9,10]

Table 22: Wyckoff bond: 4b@4e

No.	vector	center	mapping
1	$[X, -X, 0]$	$[0, 0, z]$	$[1, -2, 15, -16]$
2	$[X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, -4, 13, -14]$
3	$[-X, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[5, -6, 11, -12]$
4	$[-X, X, 0]$	$[0, 0, -z]$	$[7, -8, 9, -10]$

Table 23: Wyckoff bond: 4c@4e

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	$[1, 2, 15, 16]$
2	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, 4, 13, 14]$
3	$[0, 0, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[5, 6, 11, 12]$
4	$[0, 0, -Z]$	$[0, 0, -z]$	$[7, 8, 9, 10]$

Table 24: Wyckoff bond: 8d@4e

No.	vector	center	mapping
1	$[X, X, Z]$	$[0, 0, z]$	$[1, 16]$
2	$[-X, -X, Z]$	$[0, 0, z]$	$[2, 15]$
3	$[-X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, 14]$
4	$[X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[4, 13]$
5	$[-X, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[5, 12]$
6	$[X, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[6, 11]$
7	$[X, X, -Z]$	$[0, 0, -z]$	$[7, 10]$
8	$[-X, -X, -Z]$	$[0, 0, -z]$	$[8, 9]$

Table 25: Wyckoff bond: 8e@4e

No.	vector	center	mapping
1	$[X, -X, Z]$	$[0, 0, z]$	$[1, 15]$
2	$[-X, X, Z]$	$[0, 0, z]$	$[2, 16]$
3	$[X, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[3, 13]$
4	$[-X, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	$[4, 14]$
5	$[-X, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[5, 11]$
6	$[X, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[6, 12]$
7	$[-X, X, -Z]$	$[0, 0, -z]$	$[7, 9]$
8	$[X, -X, -Z]$	$[0, 0, -z]$	$[8, 10]$

Table 26: Wyckoff bond: 8f@4e

No.	vector	center	mapping
1	[X, Y, 0]	[0, 0, z]	[1, -2]
2	[-Y, X, 0]	[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]	[3, -4]
3	[-X, Y, 0]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[5, -6]
4	[Y, X, 0]	[0, 0, -z]	[7, -8]
5	[-X, -Y, 0]	[0, 0, -z]	[9, -10]
6	[Y, -X, 0]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[11, -12]
7	[X, -Y, 0]	[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]	[13, -14]
8	[-Y, -X, 0]	[0, 0, z]	[15, -16]

Table 27: Wyckoff bond: 16g@4e

No.	vector	center	mapping
1	[X, Y, Z]	[0, 0, z]	[1]
2	[-X, -Y, Z]	[0, 0, z]	[2]
3	[-Y, X, Z]	[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]	[3]
4	[Y, -X, Z]	[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]	[4]
5	[-X, Y, -Z]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[5]
6	[X, -Y, -Z]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[6]
7	[Y, X, -Z]	[0, 0, -z]	[7]
8	[-Y, -X, -Z]	[0, 0, -z]	[8]
9	[-X, -Y, -Z]	[0, 0, -z]	[9]
10	[X, Y, -Z]	[0, 0, -z]	[10]
11	[Y, -X, -Z]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[11]
12	[-Y, X, -Z]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[12]
13	[X, -Y, Z]	[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]	[13]
14	[-X, Y, Z]	[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]	[14]
15	[-Y, -X, Z]	[0, 0, z]	[15]
16	[Y, X, Z]	[0, 0, z]	[16]

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

Table 28: Wyckoff bond: 4a@4f

No.	vector	center	mapping
1	[X, X, 0]	[x, x, 0]	[1, 7, 10, 16]
2	[-X, -X, 0]	[-x, -x, 0]	[2, 8, 9, 15]
3	[-X, X, 0]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]	[3, 5, 12, 14]
4	[X, -X, 0]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[4, 6, 11, 13]

Table 29: Wyckoff bond: 4b@4f

No.	vector	center	mapping
1	[ $X, -X, 0$ ]	[ $x, x, 0$ ]	[1, -7, 10, -16]
2	[ $-X, X, 0$ ]	[ $-x, -x, 0$ ]	[2, -8, 9, -15]
3	[ $X, X, 0$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}$ ]	[3, -5, 12, -14]
4	[ $-X, -X, 0$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}$ ]	[4, -6, 11, -13]

Table 30: Wyckoff bond: 4c@4f

No.	vector	center	mapping
1	[0, 0, $Z$ ]	[ $x, x, 0$ ]	[1, -7, -10, 16]
2	[0, 0, $Z$ ]	[ $-x, -x, 0$ ]	[2, -8, -9, 15]
3	[0, 0, $Z$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}$ ]	[3, -5, -12, 14]
4	[0, 0, $Z$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}$ ]	[4, -6, -11, 13]

Table 31: Wyckoff bond: 8d@4f

No.	vector	center	mapping
1	[ $X, X, Z$ ]	[ $x, x, 0$ ]	[1, 16]
2	[ $-X, -X, Z$ ]	[ $-x, -x, 0$ ]	[2, 15]
3	[ $-X, X, Z$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}$ ]	[3, 14]
4	[ $X, -X, Z$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}$ ]	[4, 13]
5	[ $-X, X, -Z$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}$ ]	[5, 12]
6	[ $X, -X, -Z$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}$ ]	[6, 11]
7	[ $X, X, -Z$ ]	[ $x, x, 0$ ]	[7, 10]
8	[ $-X, -X, -Z$ ]	[ $-x, -x, 0$ ]	[8, 9]

Table 32: Wyckoff bond: 8e@4f

No.	vector	center	mapping
1	[ $X, -X, Z$ ]	[ $x, x, 0$ ]	[1, -7]
2	[ $-X, X, Z$ ]	[ $-x, -x, 0$ ]	[2, -8]
3	[ $X, X, Z$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}$ ]	[3, -5]
4	[ $-X, -X, Z$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}$ ]	[4, -6]
5	[ $-X, X, -Z$ ]	[ $-x, -x, 0$ ]	[9, -15]
6	[ $X, -X, -Z$ ]	[ $x, x, 0$ ]	[10, -16]
7	[ $-X, -X, -Z$ ]	[ $x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}$ ]	[11, -13]
8	[ $X, X, -Z$ ]	[ $\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}$ ]	[12, -14]

Table 33: Wyckoff bond: 8f@4f

No.	vector	center	mapping
1	[X, Y, 0]	[x, x, 0]	[1, 10]
2	[-X, -Y, 0]	[-x, -x, 0]	[2, 9]
3	[-Y, X, 0]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]	[3, 12]
4	[Y, -X, 0]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[4, 11]
5	[-X, Y, 0]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]	[5, 14]
6	[X, -Y, 0]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[6, 13]
7	[Y, X, 0]	[x, x, 0]	[7, 16]
8	[-Y, -X, 0]	[-x, -x, 0]	[8, 15]

Table 34: Wyckoff bond: 16g@4f

No.	vector	center	mapping
1	[X, Y, Z]	[x, x, 0]	[1]
2	[-X, -Y, Z]	[-x, -x, 0]	[2]
3	[-Y, X, Z]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]	[3]
4	[Y, -X, Z]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[4]
5	[-X, Y, -Z]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]	[5]
6	[X, -Y, -Z]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[6]
7	[Y, X, -Z]	[x, x, 0]	[7]
8	[-Y, -X, -Z]	[-x, -x, 0]	[8]
9	[-X, -Y, -Z]	[-x, -x, 0]	[9]
10	[X, Y, -Z]	[x, x, 0]	[10]
11	[Y, -X, -Z]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[11]
12	[-Y, X, -Z]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]	[12]
13	[X, -Y, Z]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[13]
14	[-X, Y, Z]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2}]	[14]
15	[-Y, -X, Z]	[-x, -x, 0]	[15]
16	[Y, X, Z]	[x, x, 0]	[16]

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

Table 35: Wyckoff bond: 4a@4g

No.	vector	center	mapping
1	[X, X, 0]	[x, -x, 0]	[1, -8, 10, -15]
2	[-X, -X, 0]	[-x, x, 0]	[2, -7, 9, -16]
3	[-X, X, 0]	[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]	[3, -6, 12, -13]
4	[X, -X, 0]	[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]	[4, -5, 11, -14]

Table 36: Wyckoff bond: 4b@4g

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, -x, 0]$	[1,8,10,15]
2	$[-X, X, 0]$	$[-x, x, 0]$	[2,7,9,16]
3	$[X, X, 0]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[3,6,12,13]
4	$[-X, -X, 0]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[4,5,11,14]

Table 37: Wyckoff bond: 4c@4g

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, -x, 0]$	[1,-8,-10,15]
2	$[0, 0, Z]$	$[-x, x, 0]$	[2,-7,-9,16]
3	$[0, 0, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[3,-6,-12,13]
4	$[0, 0, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[4,-5,-11,14]

Table 38: Wyckoff bond: 8d@4g

No.	vector	center	mapping
1	$[X, X, Z]$	$[x, -x, 0]$	[1,-8]
2	$[-X, -X, Z]$	$[-x, x, 0]$	[2,-7]
3	$[-X, X, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[3,-6]
4	$[X, -X, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[4,-5]
5	$[-X, -X, -Z]$	$[-x, x, 0]$	[9,-16]
6	$[X, X, -Z]$	$[x, -x, 0]$	[10,-15]
7	$[X, -X, -Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[11,-14]
8	$[-X, X, -Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[12,-13]

Table 39: Wyckoff bond: 8e@4g

No.	vector	center	mapping
1	$[X, -X, Z]$	$[x, -x, 0]$	[1,15]
2	$[-X, X, Z]$	$[-x, x, 0]$	[2,16]
3	$[X, X, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[3,13]
4	$[-X, -X, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[4,14]
5	$[-X, -X, -Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[5,11]
6	$[X, X, -Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[6,12]
7	$[-X, X, -Z]$	$[-x, x, 0]$	[7,9]
8	$[X, -X, -Z]$	$[x, -x, 0]$	[8,10]

Table 40: Wyckoff bond: 8f@4g

No.	vector	center	mapping
1	[X, Y, 0]	[x, -x, 0]	[1, 10]
2	[-X, -Y, 0]	[-x, x, 0]	[2, 9]
3	[-Y, X, 0]	[x + 1/2, x + 1/2, 1/2]	[3, 12]
4	[Y, -X, 0]	[1/2 - x, 1/2 - x, 1/2]	[4, 11]
5	[-X, Y, 0]	[1/2 - x, 1/2 - x, 1/2]	[5, 14]
6	[X, -Y, 0]	[x + 1/2, x + 1/2, 1/2]	[6, 13]
7	[Y, X, 0]	[-x, x, 0]	[7, 16]
8	[-Y, -X, 0]	[x, -x, 0]	[8, 15]

Table 41: Wyckoff bond: 16g@4g

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 + 1/2, x + 1/2, 1/2]	[3]
4	[Y, -X, Z]	[1/2 - x, 1/2 - x, 1/2]	[4]
5	[-X, Y, -Z]	[1/2 - x, 1/2 - x, 1/2]	[5]
6	[X, -Y, -Z]	[x + 1/2, x + 1/2, 1/2]	[6]
7	[Y, X, -Z]	[-x, x, 0]	[7]
8	[-Y, -X, -Z]	[x, -x, 0]	[8]
9	[-X, -Y, -Z]	[-x, x, 0]	[9]
10	[X, Y, -Z]	[x, -x, 0]	[10]
11	[Y, -X, -Z]	[1/2 - x, 1/2 - x, 1/2]	[11]
12	[-Y, X, -Z]	[x + 1/2, x + 1/2, 1/2]	[12]
13	[X, -Y, Z]	[x + 1/2, x + 1/2, 1/2]	[13]
14	[-X, Y, Z]	[1/2 - x, 1/2 - x, 1/2]	[14]
15	[-Y, -X, Z]	[x, -x, 0]	[15]
16	[Y, X, Z]	[-x, x, 0]	[16]

\* Wyckoff site: 8h, site symmetry: 2..

Table 42: Wyckoff bond: 8a@8h

No.	vector	center	mapping
1	[X, Y, 0]	[0, 1/2, z]	[1, -2]
2	[-Y, X, 0]	[0, 1/2, z + 1/2]	[3, -4]
3	[-X, Y, 0]	[1/2, 0, 1/2 - z]	[5, -6]
4	[Y, X, 0]	[1/2, 0, -z]	[7, -8]
5	[-X, -Y, 0]	[0, 1/2, -z]	[9, -10]
6	[Y, -X, 0]	[0, 1/2, 1/2 - z]	[11, -12]
7	[X, -Y, 0]	[1/2, 0, z + 1/2]	[13, -14]
8	[-Y, -X, 0]	[1/2, 0, z]	[15, -16]

Table 43: Wyckoff bond: 8b@8h

No.	vector	center	mapping
1	[0, 0, Z]	[0, $\frac{1}{2}$ , z]	[1, 2]
2	[0, 0, Z]	[0, $\frac{1}{2}$ , $z + \frac{1}{2}$ ]	[3, 4]
3	[0, 0, -Z]	[ $\frac{1}{2}$ , 0, $\frac{1}{2} - z$ ]	[5, 6]
4	[0, 0, -Z]	[ $\frac{1}{2}$ , 0, -z]	[7, 8]
5	[0, 0, -Z]	[0, $\frac{1}{2}$ , -z]	[9, 10]
6	[0, 0, -Z]	[0, $\frac{1}{2}$ , $\frac{1}{2} - z$ ]	[11, 12]
7	[0, 0, Z]	[ $\frac{1}{2}$ , 0, $z + \frac{1}{2}$ ]	[13, 14]
8	[0, 0, Z]	[ $\frac{1}{2}$ , 0, z]	[15, 16]

Table 44: Wyckoff bond: 16c@8h

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]	[0, $\frac{1}{2}$ , $z + \frac{1}{2}$ ]	[3]
4	[Y, -X, Z]	[0, $\frac{1}{2}$ , $z + \frac{1}{2}$ ]	[4]
5	[-X, Y, -Z]	[ $\frac{1}{2}$ , 0, $\frac{1}{2} - z$ ]	[5]
6	[X, -Y, -Z]	[ $\frac{1}{2}$ , 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]
9	[-X, -Y, -Z]	[0, $\frac{1}{2}$ , -z]	[9]
10	[X, Y, -Z]	[0, $\frac{1}{2}$ , -z]	[10]
11	[Y, -X, -Z]	[0, $\frac{1}{2}$ , $\frac{1}{2} - z$ ]	[11]
12	[-Y, X, -Z]	[0, $\frac{1}{2}$ , $\frac{1}{2} - z$ ]	[12]
13	[X, -Y, Z]	[ $\frac{1}{2}$ , 0, $z + \frac{1}{2}$ ]	[13]
14	[-X, Y, Z]	[ $\frac{1}{2}$ , 0, $z + \frac{1}{2}$ ]	[14]
15	[-Y, -X, Z]	[ $\frac{1}{2}$ , 0, z]	[15]
16	[Y, X, Z]	[ $\frac{1}{2}$ , 0, z]	[16]

\* Wyckoff site: 8i, site symmetry: m..

Table 45: Wyckoff bond: 8a@8i

No.	vector	center	mapping
1	[X, Y, 0]	[x, y, 0]	[1, 10]
2	[-X, -Y, 0]	[-x, -y, 0]	[2, 9]
3	[-Y, X, 0]	[ $\frac{1}{2} - y$ , $x + \frac{1}{2}$ , $\frac{1}{2}$ ]	[3, 12]
4	[Y, -X, 0]	[ $y + \frac{1}{2}$ , $\frac{1}{2} - x$ , $\frac{1}{2}$ ]	[4, 11]
5	[-X, Y, 0]	[ $\frac{1}{2} - x$ , $y + \frac{1}{2}$ , $\frac{1}{2}$ ]	[5, 14]
6	[X, -Y, 0]	[ $x + \frac{1}{2}$ , $\frac{1}{2} - y$ , $\frac{1}{2}$ ]	[6, 13]

*continued ...*

Table 45

No.	vector	center	mapping
7	[Y, X, 0]	[y, x, 0]	[7, 16]
8	[-Y, -X, 0]	[-y, -x, 0]	[8, 15]

Table 46: Wyckoff bond: 8b@8i

No.	vector	center	mapping
1	[0, 0, Z]	[x, y, 0]	[1, -10]
2	[0, 0, Z]	[-x, -y, 0]	[2, -9]
3	[0, 0, Z]	[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]	[3, -12]
4	[0, 0, Z]	[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[4, -11]
5	[0, 0, -Z]	[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]	[5, -14]
6	[0, 0, -Z]	[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]	[6, -13]
7	[0, 0, -Z]	[y, x, 0]	[7, -16]
8	[0, 0, -Z]	[-y, -x, 0]	[8, -15]

Table 47: Wyckoff bond: 16c@8i

No.	vector	center	mapping
1	[X, Y, Z]	[x, y, 0]	[1]
2	[-X, -Y, Z]	[-x, -y, 0]	[2]
3	[-Y, X, Z]	[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]	[3]
4	[Y, -X, Z]	[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[4]
5	[-X, Y, -Z]	[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]	[5]
6	[X, -Y, -Z]	[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]	[6]
7	[Y, X, -Z]	[y, x, 0]	[7]
8	[-Y, -X, -Z]	[-y, -x, 0]	[8]
9	[-X, -Y, -Z]	[-x, -y, 0]	[9]
10	[X, Y, -Z]	[x, y, 0]	[10]
11	[Y, -X, -Z]	[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[11]
12	[-Y, X, -Z]	[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]	[12]
13	[X, -Y, Z]	[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]	[13]
14	[-X, Y, Z]	[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]	[14]
15	[-Y, -X, Z]	[-y, -x, 0]	[15]
16	[Y, X, Z]	[y, x, 0]	[16]

\* Wyckoff site: 8j, site symmetry: . .m

Table 48: Wyckoff bond: 8a@8j

No.	vector	center	mapping
1	[X, X, Z]	[x, x, z]	[1,16]
2	[-X, -X, Z]	[-x, -x, z]	[2,15]
3	[-X, X, Z]	[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]	[3,14]
4	[X, -X, Z]	[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]	[4,13]
5	[-X, X, -Z]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - z]	[5,12]
6	[X, -X, -Z]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]	[6,11]
7	[X, X, -Z]	[x, x, -z]	[7,10]
8	[-X, -X, -Z]	[-x, -x, -z]	[8,9]

Table 49: Wyckoff bond: 8b@8j

No.	vector	center	mapping
1	[X, -X, 0]	[x, x, z]	[1,-16]
2	[-X, X, 0]	[-x, -x, z]	[2,-15]
3	[X, X, 0]	[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]	[3,-14]
4	[-X, -X, 0]	[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]	[4,-13]
5	[-X, -X, 0]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - z]	[5,-12]
6	[X, X, 0]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]	[6,-11]
7	[-X, X, 0]	[x, x, -z]	[7,-10]
8	[X, -X, 0]	[-x, -x, -z]	[8,-9]

Table 50: Wyckoff bond: 16c@8j

No.	vector	center	mapping
1	[X, Y, Z]	[x, x, z]	[1]
2	[-X, -Y, Z]	[-x, -x, z]	[2]
3	[-Y, X, Z]	[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]	[3]
4	[Y, -X, Z]	[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]	[4]
5	[-X, Y, -Z]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - z]	[5]
6	[X, -Y, -Z]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]	[6]
7	[Y, X, -Z]	[x, x, -z]	[7]
8	[-Y, -X, -Z]	[-x, -x, -z]	[8]
9	[-X, -Y, -Z]	[-x, -x, -z]	[9]
10	[X, Y, -Z]	[x, x, -z]	[10]
11	[Y, -X, -Z]	[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]	[11]
12	[-Y, X, -Z]	[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - z]	[12]
13	[X, -Y, Z]	[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]	[13]
14	[-X, Y, Z]	[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]	[14]
15	[-Y, -X, Z]	[-x, -x, z]	[15]
16	[Y, X, Z]	[x, x, z]	[16]

\* Wyckoff site: 16k, site symmetry: 1

Table 51: Wyckoff bond: 16a@16k

No.	vector	center	mapping
1	[X, Y, Z]	[x, y, z]	[1]
2	[-X, -Y, Z]	[-x, -y, z]	[2]
3	[-Y, X, Z]	[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]	[3]
4	[Y, -X, Z]	[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]	[4]
5	[-X, Y, -Z]	[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]	[5]
6	[X, -Y, -Z]	[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]	[6]
7	[Y, X, -Z]	[y, x, -z]	[7]
8	[-Y, -X, -Z]	[-y, -x, -z]	[8]
9	[-X, -Y, -Z]	[-x, -y, -z]	[9]
10	[X, Y, -Z]	[x, y, -z]	[10]
11	[Y, -X, -Z]	[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]	[11]
12	[-Y, X, -Z]	[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]	[12]
13	[X, -Y, Z]	[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]	[13]
14	[-X, Y, Z]	[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]	[14]
15	[-Y, -X, Z]	[-y, -x, z]	[15]
16	[Y, X, Z]	[y, x, z]	[16]