

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

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

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

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:  $m.mm$

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	$[-Y, X, 0]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[3, 12]
4	$[Y, -X, 0]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[4, 11]
5	$[-X, Y, 0]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[5, 14]
6	$[X, -Y, 0]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[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	$[-Y, X, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[3]
4	$[Y, -X, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[4]
5	$[-X, Y, -Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[5]
6	$[X, -Y, -Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[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	$[Y, -X, -Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[11]
12	$[-Y, X, -Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[12]
13	$[X, -Y, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2}]$	[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	$[X, Y, 0]$	$[0, \frac{1}{2}, z]$	[1, -2]
2	$[-Y, X, 0]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[3, -4]
3	$[-X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[5, -6]
4	$[Y, X, 0]$	$[\frac{1}{2}, 0, -z]$	[7, -8]
5	$[-X, -Y, 0]$	$[0, \frac{1}{2}, -z]$	[9, -10]
6	$[Y, -X, 0]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[11, -12]
7	$[X, -Y, 0]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[13, -14]
8	$[-Y, -X, 0]$	$[\frac{1}{2}, 0, z]$	[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]

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]