

SG No. 135 D_{4h}^{13} $P4_2/mbc$ [tetragonal]

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

* Wyckoff site: **4a**, site symmetry: $2/m..$

Table 1: Wyckoff bond: **4a@4a**

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

Table 2: Wyckoff bond: **4b@4a**

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

Table 3: Wyckoff bond: **8c@4a**

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

* Wyckoff site: **4b**, site symmetry: $-4..$

Table 4: Wyckoff bond: **4a@4b**

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

Table 5: Wyckoff bond: **8b@4b**

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

Table 6: Wyckoff bond: **16c@4b**

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

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

Table 7: Wyckoff bond: **4a@4c**

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

Table 8: Wyckoff bond: **4b@4c**

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

Table 9: 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	$[-Y, X, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[3, -11]$
4	$[Y, -X, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[4, -12]$
5	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, 0]$	$[5, -13]$
6	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, 0]$	$[6, -14]$
7	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[7, -15]$
8	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[8, -16]$

* Wyckoff site: **4d**, site symmetry: **2.22**

Table 10: Wyckoff bond: **4a@4d**

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

Table 11: Wyckoff bond: **4b@4d**

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

Table 12: Wyckoff bond: 4c@4d

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

Table 13: Wyckoff bond: 8d@4d

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

Table 14: Wyckoff bond: 8e@4d

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

Table 15: Wyckoff bond: 8f@4d

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

continued ...

Table 15

No.	vector	center	mapping
8	$[-Y, -X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[15,-16]

Table 16: Wyckoff bond: 16g@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	$[-Y, X, Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[3]
4	$[Y, -X, Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[4]
5	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[5]
6	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[6]
7	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[7]
8	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[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	$[Y, -X, -Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[11]
12	$[-Y, X, -Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[12]
13	$[X, -Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[13]
14	$[-X, Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[14]
15	$[-Y, -X, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[15]
16	$[Y, X, Z]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[16]

* Wyckoff site: 8e, site symmetry: 2..

Table 17: Wyckoff bond: 8a@8e

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

Table 18: Wyckoff bond: 8b@8e

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

continued ...

Table 18

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

Table 19: Wyckoff bond: **16c@8e**

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

* Wyckoff site: **8f**, site symmetry: **2..**

Table 20: Wyckoff bond: **8a@8f**

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

Table 21: Wyckoff bond: **8b@8f**

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

Table 22: Wyckoff bond: **16c@8f**

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	$[-Y, X, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[3]$
4	$[Y, -X, Z]$	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	$[4]$
5	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, -z]$	$[5]$
6	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, -z]$	$[6]$
7	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	$[7]$
8	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2} - z]$	$[8]$
9	$[-X, -Y, -Z]$	$[0, \frac{1}{2}, -z]$	$[9]$
10	$[X, Y, -Z]$	$[0, \frac{1}{2}, -z]$	$[10]$
11	$[Y, -X, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	$[11]$
12	$[-Y, X, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	$[12]$
13	$[X, -Y, Z]$	$[\frac{1}{2}, 0, z]$	$[13]$
14	$[-X, Y, Z]$	$[\frac{1}{2}, 0, z]$	$[14]$
15	$[-Y, -X, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[15]$
16	$[Y, X, Z]$	$[0, \frac{1}{2}, z + \frac{1}{2}]$	$[16]$

* Wyckoff site: **8g**, site symmetry: $\dots 2$

Table 23: Wyckoff bond: **8a@8g**

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

Table 24: Wyckoff bond: **8b@8g**

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

Table 25: Wyckoff bond: **16c@8g**

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

* Wyckoff site: **8h**, site symmetry: **m** . .

Table 26: Wyckoff bond: **8a@8h**

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

continued ...

Table 26

No.	vector	center	mapping
7	$[Y, X, 0]$	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[7, 16]$
8	$[-Y, -X, 0]$	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2}]$	$[8, 15]$

Table 27: Wyckoff bond: **8b@8h**

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

Table 28: Wyckoff bond: **16c@8h**

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

* Wyckoff site: **16i**, site symmetry: **1**

Table 29: Wyckoff bond: **16a@16i**

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