

SG No. 125 D_{4h}^3 $P4/nbm$ [tetragonal]

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

* Wyckoff site: 2a, site symmetry: 422

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 4b@2a

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

Table 3: Wyckoff bond: 4c@2a

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

Table 4: Wyckoff bond: 8d@2a

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

Table 5: Wyckoff bond: 8e@2a

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

Table 6: Wyckoff bond: 8f@2a

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

Table 7: Wyckoff bond: 16g@2a

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

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 4b@2b

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

Table 10: Wyckoff bond: 4c@2b

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

Table 11: Wyckoff bond: 8d@2b

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

Table 12: Wyckoff bond: **8e@2b**

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

Table 13: Wyckoff bond: **8f@2b**

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

Table 14: Wyckoff bond: **16g@2b**

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

Table 15: Wyckoff bond: 2a@2c

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

Table 16: Wyckoff bond: 4b@2c

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

Table 17: Wyckoff bond: 4c@2c

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

Table 18: Wyckoff bond: 8d@2c

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

Table 19: Wyckoff bond: $8e@2c$

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

Table 20: Wyckoff bond: $8f@2c$

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

Table 21: Wyckoff bond: $16g@2c$

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

Table 22: Wyckoff bond: 2a@2d

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

Table 23: Wyckoff bond: 4b@2d

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

Table 24: Wyckoff bond: 4c@2d

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

Table 25: Wyckoff bond: 8d@2d

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

Table 26: Wyckoff bond: $8e@2d$

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

Table 27: Wyckoff bond: $8f@2d$

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

Table 28: Wyckoff bond: $16g@2d$

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

* Wyckoff site: **4e**, site symmetry: \dots/m

Table 29: Wyckoff bond: **4a@4e**

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

Table 30: Wyckoff bond: **4b@4e**

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

Table 31: Wyckoff bond: **8c@4e**

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

* Wyckoff site: **4f**, site symmetry: \dots/m

Table 32: Wyckoff bond: **4a@4f**

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

Table 33: Wyckoff bond: 4b@4f

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

Table 34: Wyckoff bond: 8c@4f

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

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

Table 35: Wyckoff bond: 4a@4g

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

Table 36: Wyckoff bond: 8b@4g

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

Table 37: Wyckoff bond: 16c@4g

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

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

Table 38: Wyckoff bond: 4a@4h

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

Table 39: Wyckoff bond: 4b@4h

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

Table 40: Wyckoff bond: 8c@4h

No.	vector	center	mapping
1	$[X, X, Z]$	$[\frac{3}{4}, \frac{1}{4}, z]$	[1, 16]

continued ...

Table 40

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

Table 41: Wyckoff bond: **8d@4h**

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

Table 42: Wyckoff bond: **16e@4h**

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

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

Table 43: Wyckoff bond: **8a@8i**

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

Table 44: Wyckoff bond: **8b@8i**

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

Table 45: Wyckoff bond: **16c@8i**

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

Table 46: Wyckoff bond: 8a@8j

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

Table 47: Wyckoff bond: 8b@8j

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

Table 48: Wyckoff bond: 16c@8j

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

continued ...

Table 48

No.	vector	center	mapping
16	$[Y, X, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[16]

* Wyckoff site: $8k$, site symmetry: $.2$.

Table 49: Wyckoff bond: $8a@8k$

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

Table 50: Wyckoff bond: $8b@8k$

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

Table 51: Wyckoff bond: $16c@8k$

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, \frac{1}{4}, 0]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, \frac{1}{4}, 0]$	[2]
3	$[-Y, X, Z]$	$[\frac{1}{4}, x, 0]$	[3]
4	$[Y, -X, Z]$	$[\frac{1}{4}, \frac{1}{2} - x, 0]$	[4]
5	$[-X, Y, -Z]$	$[\frac{1}{2} - x, \frac{1}{4}, 0]$	[5]
6	$[X, -Y, -Z]$	$[x, \frac{1}{4}, 0]$	[6]
7	$[Y, X, -Z]$	$[\frac{1}{4}, x, 0]$	[7]
8	$[-Y, -X, -Z]$	$[\frac{1}{4}, \frac{1}{2} - x, 0]$	[8]
9	$[-X, -Y, -Z]$	$[-x, \frac{3}{4}, 0]$	[9]

continued ...

Table 51

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

* Wyckoff site: 81, site symmetry: .2.

Table 52: Wyckoff bond: 8a@81

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

Table 53: Wyckoff bond: 8b@81

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

Table 54: Wyckoff bond: 16c@81

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

continued ...

Table 54

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

* Wyckoff site: 8m, site symmetry: $\dots m$

Table 55: Wyckoff bond: 8a@8m

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

Table 56: Wyckoff bond: 8b@8m

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

Table 57: Wyckoff bond: 16c@8m

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

* Wyckoff site: 16n, site symmetry: 1

Table 58: Wyckoff bond: 16a@16n

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