

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:  $\dots 2/m$

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:  $\dots 2/m$

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:  $\bar{3}m$

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]