

# SG No. 215 $T_d^1$ $P\bar{4}3m$ [ cubic ]

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

\* Wyckoff site: **1a**, site symmetry:  $-43m$

Table 1: Wyckoff bond: **3a@1a**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, 0]$	$[1, -2, -3, 4, 17, -18, -19, 20]$
2	$[0, X, 0]$	$[0, 0, 0]$	$[5, -6, -7, 8, 13, -14, -15, 16]$
3	$[0, 0, X]$	$[0, 0, 0]$	$[9, -10, -11, 12, 21, -22, -23, 24]$

Table 2: Wyckoff bond: **4b@1a**

No.	vector	center	mapping
1	$[X, X, X]$	$[0, 0, 0]$	$[1, 5, 9, 13, 17, 21]$
2	$[-X, -X, X]$	$[0, 0, 0]$	$[2, 7, 12, 14, 19, 24]$
3	$[-X, X, -X]$	$[0, 0, 0]$	$[3, 8, 10, 16, 18, 23]$
4	$[X, -X, -X]$	$[0, 0, 0]$	$[4, 6, 11, 15, 20, 22]$

Table 3: Wyckoff bond: **6c@1a**

No.	vector	center	mapping
1	$[X, X, 0]$	$[0, 0, 0]$	$[1, -2, 13, -14]$
2	$[-X, X, 0]$	$[0, 0, 0]$	$[3, -4, -15, 16]$
3	$[0, X, X]$	$[0, 0, 0]$	$[5, -6, 21, -22]$
4	$[0, -X, X]$	$[0, 0, 0]$	$[7, -8, -23, 24]$
5	$[X, 0, X]$	$[0, 0, 0]$	$[9, -10, 17, -18]$
6	$[X, 0, -X]$	$[0, 0, 0]$	$[11, -12, -19, 20]$

Table 4: Wyckoff bond: **12d@1a**

No.	vector	center	mapping
1	$[X, X, Y]$	$[0, 0, 0]$	$[1, 13]$
2	$[-X, -X, Y]$	$[0, 0, 0]$	$[2, 14]$
3	$[-X, X, -Y]$	$[0, 0, 0]$	$[3, 16]$
4	$[X, -X, -Y]$	$[0, 0, 0]$	$[4, 15]$
5	$[Y, X, X]$	$[0, 0, 0]$	$[5, 21]$
6	$[Y, -X, -X]$	$[0, 0, 0]$	$[6, 22]$
7	$[-Y, -X, X]$	$[0, 0, 0]$	$[7, 24]$
8	$[-Y, X, -X]$	$[0, 0, 0]$	$[8, 23]$
9	$[X, Y, X]$	$[0, 0, 0]$	$[9, 17]$
10	$[-X, Y, -X]$	$[0, 0, 0]$	$[10, 18]$

*continued ...*

Table 4

No.	vector	center	mapping
11	$[X, -Y, -X]$	$[0, 0, 0]$	$[11, 20]$
12	$[-X, -Y, X]$	$[0, 0, 0]$	$[12, 19]$

Table 5: Wyckoff bond: 12e@1a

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, 0, 0]$	$[3, -4]$
3	$[0, X, Y]$	$[0, 0, 0]$	$[5, -6]$
4	$[0, -X, Y]$	$[0, 0, 0]$	$[7, -8]$
5	$[Y, 0, X]$	$[0, 0, 0]$	$[9, -10]$
6	$[Y, 0, -X]$	$[0, 0, 0]$	$[11, -12]$
7	$[Y, X, 0]$	$[0, 0, 0]$	$[13, -14]$
8	$[Y, -X, 0]$	$[0, 0, 0]$	$[15, -16]$
9	$[X, 0, Y]$	$[0, 0, 0]$	$[17, -18]$
10	$[-X, 0, Y]$	$[0, 0, 0]$	$[19, -20]$
11	$[0, Y, X]$	$[0, 0, 0]$	$[21, -22]$
12	$[0, Y, -X]$	$[0, 0, 0]$	$[23, -24]$

Table 6: Wyckoff bond: 24f@1a

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[0, 0, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[0, 0, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[0, 0, 0]$	$[4]$
5	$[Z, X, Y]$	$[0, 0, 0]$	$[5]$
6	$[Z, -X, -Y]$	$[0, 0, 0]$	$[6]$
7	$[-Z, -X, Y]$	$[0, 0, 0]$	$[7]$
8	$[-Z, X, -Y]$	$[0, 0, 0]$	$[8]$
9	$[Y, Z, X]$	$[0, 0, 0]$	$[9]$
10	$[-Y, Z, -X]$	$[0, 0, 0]$	$[10]$
11	$[Y, -Z, -X]$	$[0, 0, 0]$	$[11]$
12	$[-Y, -Z, X]$	$[0, 0, 0]$	$[12]$
13	$[Y, X, Z]$	$[0, 0, 0]$	$[13]$
14	$[-Y, -X, Z]$	$[0, 0, 0]$	$[14]$
15	$[Y, -X, -Z]$	$[0, 0, 0]$	$[15]$
16	$[-Y, X, -Z]$	$[0, 0, 0]$	$[16]$
17	$[X, Z, Y]$	$[0, 0, 0]$	$[17]$
18	$[-X, Z, -Y]$	$[0, 0, 0]$	$[18]$
19	$[-X, -Z, Y]$	$[0, 0, 0]$	$[19]$
20	$[X, -Z, -Y]$	$[0, 0, 0]$	$[20]$

*continued ...*

Table 6

No.	vector	center	mapping
21	$[Z, Y, X]$	$[0, 0, 0]$	$[21]$
22	$[Z, -Y, -X]$	$[0, 0, 0]$	$[22]$
23	$[-Z, Y, -X]$	$[0, 0, 0]$	$[23]$
24	$[-Z, -Y, X]$	$[0, 0, 0]$	$[24]$

\* Wyckoff site: **1b**, site symmetry: **-43m**

Table 7: Wyckoff bond: **3a@1b**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -3, 4, 17, -18, -19, 20]$
2	$[0, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[5, -6, -7, 8, 13, -14, -15, 16]$
3	$[0, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[9, -10, -11, 12, 21, -22, -23, 24]$

Table 8: Wyckoff bond: **4b@1b**

No.	vector	center	mapping
1	$[X, X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 5, 9, 13, 17, 21]$
2	$[-X, -X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 7, 12, 14, 19, 24]$
3	$[-X, X, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, 8, 10, 16, 18, 23]$
4	$[X, -X, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[4, 6, 11, 15, 20, 22]$

Table 9: Wyckoff bond: **6c@1b**

No.	vector	center	mapping
1	$[X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, 13, -14]$
2	$[-X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, -4, -15, 16]$
3	$[0, X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[5, -6, 21, -22]$
4	$[0, -X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[7, -8, -23, 24]$
5	$[X, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[9, -10, 17, -18]$
6	$[X, 0, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[11, -12, -19, 20]$

Table 10: Wyckoff bond: **12d@1b**

No.	vector	center	mapping
1	$[X, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 13]$
2	$[-X, -X, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, 14]$
3	$[-X, X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, 16]$

*continued ...*

Table 10

No.	vector	center	mapping
4	$[X, -X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[4,15]
5	$[Y, X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[5,21]
6	$[Y, -X, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[6,22]
7	$[-Y, -X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[7,24]
8	$[-Y, X, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[8,23]
9	$[X, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9,17]
10	$[-X, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[10,18]
11	$[X, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[11,20]
12	$[-X, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[12,19]

Table 11: Wyckoff bond: **12e@1b**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1,-2]
2	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[3,-4]
3	$[0, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[5,-6]
4	$[0, -X, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[7,-8]
5	$[Y, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9,-10]
6	$[Y, 0, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[11,-12]
7	$[Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[13,-14]
8	$[Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[15,-16]
9	$[X, 0, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[17,-18]
10	$[-X, 0, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[19,-20]
11	$[0, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[21,-22]
12	$[0, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[23,-24]

Table 12: Wyckoff bond: **24f@1b**

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

*continued ...*

Table 12

No.	vector	center	mapping
14	$[-Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[14]
15	$[Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[15]
16	$[-Y, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[16]
17	$[X, Z, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[17]
18	$[-X, Z, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[18]
19	$[-X, -Z, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[19]
20	$[X, -Z, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[20]
21	$[Z, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[21]
22	$[Z, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[22]
23	$[-Z, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[23]
24	$[-Z, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[24]

\* Wyckoff site: 3c, site symmetry:  $-42.m$

Table 13: Wyckoff bond: 3a@3c

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -3, 4, 17, -18, -19, 20]$
2	$[0, X, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6, -7, 8, 13, -14, -15, 16]$
3	$[0, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -10, -11, 12, 21, -22, -23, 24]$

Table 14: Wyckoff bond: 6b@3c

No.	vector	center	mapping
1	$[0, X, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -4, 17, -20]$
2	$[0, -X, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -3, -18, 19]$
3	$[X, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -8, 13, -16]$
4	$[X, 0, -X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, -7, -14, 15]$
5	$[X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -12, 21, -24]$
6	$[-X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[10, -11, -22, 23]$

Table 15: Wyckoff bond: 6c@3c

No.	vector	center	mapping
1	$[0, 0, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, -3, -4]$
2	$[X, 0, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, 6, -7, -8]$
3	$[0, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10, -11, -12]$
4	$[0, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[13, 14, -15, -16]$
5	$[0, X, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[17, 18, -19, -20]$
6	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[21, 22, -23, -24]$

Table 16: Wyckoff bond: 12d@3c

No.	vector	center	mapping
1	$[Y, X, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 17]$
2	$[-Y, -X, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, 19]$
3	$[-Y, X, -X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, 18]$
4	$[Y, -X, -X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[4, 20]$
5	$[X, Y, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, 13]$
6	$[X, -Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, 15]$
7	$[-X, -Y, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[7, 14]$
8	$[-X, Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[8, 16]$
9	$[X, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 21]$
10	$[-X, X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[10, 23]$
11	$[X, -X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[11, 22]$
12	$[-X, -X, Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[12, 24]$

Table 17: Wyckoff bond: 12e@3c

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -4]$
3	$[0, X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6]$
4	$[0, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[7, -8]$
5	$[Y, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -10]$
6	$[Y, 0, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[11, -12]$
7	$[Y, X, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[13, -14]$
8	$[Y, -X, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[15, -16]$
9	$[X, 0, Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[17, -18]$
10	$[-X, 0, Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[19, -20]$
11	$[0, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[21, -22]$
12	$[0, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[23, -24]$

Table 18: Wyckoff bond: 12f@3c

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

continued ...

Table 18

No.	vector	center	mapping
8	$[-X, 0, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[14,-15]
9	$[0, Y, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[17,-20]
10	$[0, Y, -X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[18,-19]
11	$[Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[21,-24]
12	$[Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[22,-23]

Table 19: Wyckoff bond: 24g@3c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[1]
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[2]
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[3]
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[4]
5	$[Z, X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[5]
6	$[Z, -X, -Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[6]
7	$[-Z, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[7]
8	$[-Z, X, -Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[8]
9	$[Y, Z, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[9]
10	$[-Y, Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[10]
11	$[Y, -Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[12]
13	$[Y, X, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[14]
15	$[Y, -X, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[15]
16	$[-Y, X, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[16]
17	$[X, Z, Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[17]
18	$[-X, Z, -Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[18]
19	$[-X, -Z, Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[19]
20	$[X, -Z, -Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[20]
21	$[Z, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[21]
22	$[Z, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[22]
23	$[-Z, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[23]
24	$[-Z, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	[24]

\* Wyckoff site: 3d, site symmetry:  $-42.m$

Table 20: Wyckoff bond: 3a@3d

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, 0, 0]$	[1,-2,-3,4,17,-18,-19,20]
2	$[0, X, 0]$	$[0, \frac{1}{2}, 0]$	[5,-6,-7,8,13,-14,-15,16]
3	$[0, 0, X]$	$[0, 0, \frac{1}{2}]$	[9,-10,-11,12,21,-22,-23,24]

Table 21: Wyckoff bond: 6b@3d

No.	vector	center	mapping
1	$[0, X, X]$	$[\frac{1}{2}, 0, 0]$	$[1, -4, 17, -20]$
2	$[0, -X, X]$	$[\frac{1}{2}, 0, 0]$	$[2, -3, -18, 19]$
3	$[X, 0, X]$	$[0, \frac{1}{2}, 0]$	$[5, -8, 13, -16]$
4	$[X, 0, -X]$	$[0, \frac{1}{2}, 0]$	$[6, -7, -14, 15]$
5	$[X, X, 0]$	$[0, 0, \frac{1}{2}]$	$[9, -12, 21, -24]$
6	$[-X, X, 0]$	$[0, 0, \frac{1}{2}]$	$[10, -11, -22, 23]$

Table 22: Wyckoff bond: 6c@3d

No.	vector	center	mapping
1	$[0, 0, X]$	$[\frac{1}{2}, 0, 0]$	$[1, 2, -3, -4]$
2	$[X, 0, 0]$	$[0, \frac{1}{2}, 0]$	$[5, 6, -7, -8]$
3	$[0, X, 0]$	$[0, 0, \frac{1}{2}]$	$[9, 10, -11, -12]$
4	$[0, 0, X]$	$[0, \frac{1}{2}, 0]$	$[13, 14, -15, -16]$
5	$[0, X, 0]$	$[\frac{1}{2}, 0, 0]$	$[17, 18, -19, -20]$
6	$[X, 0, 0]$	$[0, 0, \frac{1}{2}]$	$[21, 22, -23, -24]$

Table 23: Wyckoff bond: 12d@3d

No.	vector	center	mapping
1	$[Y, X, X]$	$[\frac{1}{2}, 0, 0]$	$[1, 17]$
2	$[-Y, -X, X]$	$[\frac{1}{2}, 0, 0]$	$[2, 19]$
3	$[-Y, X, -X]$	$[\frac{1}{2}, 0, 0]$	$[3, 18]$
4	$[Y, -X, -X]$	$[\frac{1}{2}, 0, 0]$	$[4, 20]$
5	$[X, Y, X]$	$[0, \frac{1}{2}, 0]$	$[5, 13]$
6	$[X, -Y, -X]$	$[0, \frac{1}{2}, 0]$	$[6, 15]$
7	$[-X, -Y, X]$	$[0, \frac{1}{2}, 0]$	$[7, 14]$
8	$[-X, Y, -X]$	$[0, \frac{1}{2}, 0]$	$[8, 16]$
9	$[X, X, Y]$	$[0, 0, \frac{1}{2}]$	$[9, 21]$
10	$[-X, X, -Y]$	$[0, 0, \frac{1}{2}]$	$[10, 23]$
11	$[X, -X, -Y]$	$[0, 0, \frac{1}{2}]$	$[11, 22]$
12	$[-X, -X, Y]$	$[0, 0, \frac{1}{2}]$	$[12, 24]$

Table 24: Wyckoff bond: 12e@3d

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

*continued ...*



Table 24

No.	vector	center	mapping
4	$[0, -X, Y]$	$[0, \frac{1}{2}, 0]$	$[7, -8]$
5	$[Y, 0, X]$	$[0, 0, \frac{1}{2}]$	$[9, -10]$
6	$[Y, 0, -X]$	$[0, 0, \frac{1}{2}]$	$[11, -12]$
7	$[Y, X, 0]$	$[0, \frac{1}{2}, 0]$	$[13, -14]$
8	$[Y, -X, 0]$	$[0, \frac{1}{2}, 0]$	$[15, -16]$
9	$[X, 0, Y]$	$[\frac{1}{2}, 0, 0]$	$[17, -18]$
10	$[-X, 0, Y]$	$[\frac{1}{2}, 0, 0]$	$[19, -20]$
11	$[0, Y, X]$	$[0, 0, \frac{1}{2}]$	$[21, -22]$
12	$[0, Y, -X]$	$[0, 0, \frac{1}{2}]$	$[23, -24]$

Table 25: Wyckoff bond: **12f03d**

No.	vector	center	mapping
1	$[0, X, Y]$	$[\frac{1}{2}, 0, 0]$	$[1, -4]$
2	$[0, -X, Y]$	$[\frac{1}{2}, 0, 0]$	$[2, -3]$
3	$[Y, 0, X]$	$[0, \frac{1}{2}, 0]$	$[5, -8]$
4	$[Y, 0, -X]$	$[0, \frac{1}{2}, 0]$	$[6, -7]$
5	$[X, Y, 0]$	$[0, 0, \frac{1}{2}]$	$[9, -12]$
6	$[-X, Y, 0]$	$[0, 0, \frac{1}{2}]$	$[10, -11]$
7	$[X, 0, Y]$	$[0, \frac{1}{2}, 0]$	$[13, -16]$
8	$[-X, 0, Y]$	$[0, \frac{1}{2}, 0]$	$[14, -15]$
9	$[0, Y, X]$	$[\frac{1}{2}, 0, 0]$	$[17, -20]$
10	$[0, Y, -X]$	$[\frac{1}{2}, 0, 0]$	$[18, -19]$
11	$[Y, X, 0]$	$[0, 0, \frac{1}{2}]$	$[21, -24]$
12	$[Y, -X, 0]$	$[0, 0, \frac{1}{2}]$	$[22, -23]$

Table 26: Wyckoff bond: **24g03d**

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

*continued ...*

Table 26

No.	vector	center	mapping
14	$[-Y, -X, Z]$	$[0, \frac{1}{2}, 0]$	[14]
15	$[Y, -X, -Z]$	$[0, \frac{1}{2}, 0]$	[15]
16	$[-Y, X, -Z]$	$[0, \frac{1}{2}, 0]$	[16]
17	$[X, Z, Y]$	$[\frac{1}{2}, 0, 0]$	[17]
18	$[-X, Z, -Y]$	$[\frac{1}{2}, 0, 0]$	[18]
19	$[-X, -Z, Y]$	$[\frac{1}{2}, 0, 0]$	[19]
20	$[X, -Z, -Y]$	$[\frac{1}{2}, 0, 0]$	[20]
21	$[Z, Y, X]$	$[0, 0, \frac{1}{2}]$	[21]
22	$[Z, -Y, -X]$	$[0, 0, \frac{1}{2}]$	[22]
23	$[-Z, Y, -X]$	$[0, 0, \frac{1}{2}]$	[23]
24	$[-Z, -Y, X]$	$[0, 0, \frac{1}{2}]$	[24]

\* Wyckoff site: **4e**, site symmetry: **.3m**

Table 27: Wyckoff bond: **4a@4e**

No.	vector	center	mapping
1	$[X, X, X]$	$[x, x, x]$	[1,5,9,13,17,21]
2	$[-X, -X, X]$	$[-x, -x, x]$	[2,7,12,14,19,24]
3	$[-X, X, -X]$	$[-x, x, -x]$	[3,8,10,16,18,23]
4	$[X, -X, -X]$	$[x, -x, -x]$	[4,6,11,15,20,22]

Table 28: Wyckoff bond: **12b@4e**

No.	vector	center	mapping
1	$[X, X, Y]$	$[x, x, x]$	[1,13]
2	$[-X, -X, Y]$	$[-x, -x, x]$	[2,14]
3	$[-X, X, -Y]$	$[-x, x, -x]$	[3,16]
4	$[X, -X, -Y]$	$[x, -x, -x]$	[4,15]
5	$[Y, X, X]$	$[x, x, x]$	[5,21]
6	$[Y, -X, -X]$	$[x, -x, -x]$	[6,22]
7	$[-Y, -X, X]$	$[-x, -x, x]$	[7,24]
8	$[-Y, X, -X]$	$[-x, x, -x]$	[8,23]
9	$[X, Y, X]$	$[x, x, x]$	[9,17]
10	$[-X, Y, -X]$	$[-x, x, -x]$	[10,18]
11	$[X, -Y, -X]$	$[x, -x, -x]$	[11,20]
12	$[-X, -Y, X]$	$[-x, -x, x]$	[12,19]

Table 29: Wyckoff bond: 12c@4e

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, x]$	$[1, -13]$
2	$[-X, X, 0]$	$[-x, -x, x]$	$[2, -14]$
3	$[-X, -X, 0]$	$[-x, x, -x]$	$[3, -16]$
4	$[X, X, 0]$	$[x, -x, -x]$	$[4, -15]$
5	$[0, X, -X]$	$[x, x, x]$	$[5, -21]$
6	$[0, -X, X]$	$[x, -x, -x]$	$[6, -22]$
7	$[0, -X, -X]$	$[-x, -x, x]$	$[7, -24]$
8	$[0, X, X]$	$[-x, x, -x]$	$[8, -23]$
9	$[-X, 0, X]$	$[x, x, x]$	$[9, -17]$
10	$[X, 0, -X]$	$[-x, x, -x]$	$[10, -18]$
11	$[-X, 0, -X]$	$[x, -x, -x]$	$[11, -20]$
12	$[X, 0, X]$	$[-x, -x, x]$	$[12, -19]$

Table 30: Wyckoff bond: 24d@4e

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, x]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, -x, x]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, x, -x]$	$[3]$
4	$[X, -Y, -Z]$	$[x, -x, -x]$	$[4]$
5	$[Z, X, Y]$	$[x, x, x]$	$[5]$
6	$[Z, -X, -Y]$	$[x, -x, -x]$	$[6]$
7	$[-Z, -X, Y]$	$[-x, -x, x]$	$[7]$
8	$[-Z, X, -Y]$	$[-x, x, -x]$	$[8]$
9	$[Y, Z, X]$	$[x, x, x]$	$[9]$
10	$[-Y, Z, -X]$	$[-x, x, -x]$	$[10]$
11	$[Y, -Z, -X]$	$[x, -x, -x]$	$[11]$
12	$[-Y, -Z, X]$	$[-x, -x, x]$	$[12]$
13	$[Y, X, Z]$	$[x, x, x]$	$[13]$
14	$[-Y, -X, Z]$	$[-x, -x, x]$	$[14]$
15	$[Y, -X, -Z]$	$[x, -x, -x]$	$[15]$
16	$[-Y, X, -Z]$	$[-x, x, -x]$	$[16]$
17	$[X, Z, Y]$	$[x, x, x]$	$[17]$
18	$[-X, Z, -Y]$	$[-x, x, -x]$	$[18]$
19	$[-X, -Z, Y]$	$[-x, -x, x]$	$[19]$
20	$[X, -Z, -Y]$	$[x, -x, -x]$	$[20]$
21	$[Z, Y, X]$	$[x, x, x]$	$[21]$
22	$[Z, -Y, -X]$	$[x, -x, -x]$	$[22]$
23	$[-Z, Y, -X]$	$[-x, x, -x]$	$[23]$
24	$[-Z, -Y, X]$	$[-x, -x, x]$	$[24]$

\* Wyckoff site: 6f, site symmetry: 2.mm

Table 31: Wyckoff bond: 6a@6f

No.	vector	center	mapping
1	$[0, X, X]$	$[x, 0, 0]$	$[1, -4, 17, -20]$
2	$[0, -X, X]$	$[-x, 0, 0]$	$[2, -3, -18, 19]$
3	$[X, 0, X]$	$[0, x, 0]$	$[5, -8, 13, -16]$
4	$[X, 0, -X]$	$[0, -x, 0]$	$[6, -7, -14, 15]$
5	$[X, X, 0]$	$[0, 0, x]$	$[9, -12, 21, -24]$
6	$[-X, X, 0]$	$[0, 0, -x]$	$[10, -11, -22, 23]$

Table 32: Wyckoff bond: 6b@6f

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	$[1, 4, 17, 20]$
2	$[-X, 0, 0]$	$[-x, 0, 0]$	$[2, 3, 18, 19]$
3	$[0, X, 0]$	$[0, x, 0]$	$[5, 8, 13, 16]$
4	$[0, -X, 0]$	$[0, -x, 0]$	$[6, 7, 14, 15]$
5	$[0, 0, X]$	$[0, 0, x]$	$[9, 12, 21, 24]$
6	$[0, 0, -X]$	$[0, 0, -x]$	$[10, 11, 22, 23]$

Table 33: Wyckoff bond: 12c@6f

No.	vector	center	mapping
1	$[Y, X, X]$	$[x, 0, 0]$	$[1, 17]$
2	$[-Y, -X, X]$	$[-x, 0, 0]$	$[2, 19]$
3	$[-Y, X, -X]$	$[-x, 0, 0]$	$[3, 18]$
4	$[Y, -X, -X]$	$[x, 0, 0]$	$[4, 20]$
5	$[X, Y, X]$	$[0, x, 0]$	$[5, 13]$
6	$[X, -Y, -X]$	$[0, -x, 0]$	$[6, 15]$
7	$[-X, -Y, X]$	$[0, -x, 0]$	$[7, 14]$
8	$[-X, Y, -X]$	$[0, x, 0]$	$[8, 16]$
9	$[X, X, Y]$	$[0, 0, x]$	$[9, 21]$
10	$[-X, X, -Y]$	$[0, 0, -x]$	$[10, 23]$
11	$[X, -X, -Y]$	$[0, 0, -x]$	$[11, 22]$
12	$[-X, -X, Y]$	$[0, 0, x]$	$[12, 24]$

Table 34: Wyckoff bond: 12d@6f

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, 0, 0]$	$[1, -4]$
2	$[0, -X, Y]$	$[-x, 0, 0]$	$[2, -3]$
3	$[Y, 0, X]$	$[0, x, 0]$	$[5, -8]$

*continued ...*

Table 34

No.	vector	center	mapping
4	$[Y, 0, -X]$	$[0, -x, 0]$	$[6, -7]$
5	$[X, Y, 0]$	$[0, 0, x]$	$[9, -12]$
6	$[-X, Y, 0]$	$[0, 0, -x]$	$[10, -11]$
7	$[X, 0, Y]$	$[0, x, 0]$	$[13, -16]$
8	$[-X, 0, Y]$	$[0, -x, 0]$	$[14, -15]$
9	$[0, Y, X]$	$[x, 0, 0]$	$[17, -20]$
10	$[0, Y, -X]$	$[-x, 0, 0]$	$[18, -19]$
11	$[Y, X, 0]$	$[0, 0, x]$	$[21, -24]$
12	$[Y, -X, 0]$	$[0, 0, -x]$	$[22, -23]$

Table 35: Wyckoff bond: **24e06f**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, 0, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, 0, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[x, 0, 0]$	$[4]$
5	$[Z, X, Y]$	$[0, x, 0]$	$[5]$
6	$[Z, -X, -Y]$	$[0, -x, 0]$	$[6]$
7	$[-Z, -X, Y]$	$[0, -x, 0]$	$[7]$
8	$[-Z, X, -Y]$	$[0, x, 0]$	$[8]$
9	$[Y, Z, X]$	$[0, 0, x]$	$[9]$
10	$[-Y, Z, -X]$	$[0, 0, -x]$	$[10]$
11	$[Y, -Z, -X]$	$[0, 0, -x]$	$[11]$
12	$[-Y, -Z, X]$	$[0, 0, x]$	$[12]$
13	$[Y, X, Z]$	$[0, x, 0]$	$[13]$
14	$[-Y, -X, Z]$	$[0, -x, 0]$	$[14]$
15	$[Y, -X, -Z]$	$[0, -x, 0]$	$[15]$
16	$[-Y, X, -Z]$	$[0, x, 0]$	$[16]$
17	$[X, Z, Y]$	$[x, 0, 0]$	$[17]$
18	$[-X, Z, -Y]$	$[-x, 0, 0]$	$[18]$
19	$[-X, -Z, Y]$	$[-x, 0, 0]$	$[19]$
20	$[X, -Z, -Y]$	$[x, 0, 0]$	$[20]$
21	$[Z, Y, X]$	$[0, 0, x]$	$[21]$
22	$[Z, -Y, -X]$	$[0, 0, -x]$	$[22]$
23	$[-Z, Y, -X]$	$[0, 0, -x]$	$[23]$
24	$[-Z, -Y, X]$	$[0, 0, x]$	$[24]$

\* Wyckoff site: **6g**, site symmetry: **2.mm**

Table 36: Wyckoff bond: 6a@6g

No.	vector	center	mapping
1	$[0, X, X]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, -4, 17, -20]$
2	$[0, -X, X]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, -3, -18, 19]$
3	$[X, 0, X]$	$[\frac{1}{2}, x, \frac{1}{2}]$	$[5, -8, 13, -16]$
4	$[X, 0, -X]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	$[6, -7, -14, 15]$
5	$[X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, x]$	$[9, -12, 21, -24]$
6	$[-X, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	$[10, -11, -22, 23]$

Table 37: Wyckoff bond: 6b@6g

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, 4, 17, 20]$
2	$[-X, 0, 0]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, 3, 18, 19]$
3	$[0, X, 0]$	$[\frac{1}{2}, x, \frac{1}{2}]$	$[5, 8, 13, 16]$
4	$[0, -X, 0]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	$[6, 7, 14, 15]$
5	$[0, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, x]$	$[9, 12, 21, 24]$
6	$[0, 0, -X]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	$[10, 11, 22, 23]$

Table 38: Wyckoff bond: 12c@6g

No.	vector	center	mapping
1	$[Y, X, X]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, 17]$
2	$[-Y, -X, X]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, 19]$
3	$[-Y, X, -X]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[3, 18]$
4	$[Y, -X, -X]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[4, 20]$
5	$[X, Y, X]$	$[\frac{1}{2}, x, \frac{1}{2}]$	$[5, 13]$
6	$[X, -Y, -X]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	$[6, 15]$
7	$[-X, -Y, X]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	$[7, 14]$
8	$[-X, Y, -X]$	$[\frac{1}{2}, x, \frac{1}{2}]$	$[8, 16]$
9	$[X, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, x]$	$[9, 21]$
10	$[-X, X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	$[10, 23]$
11	$[X, -X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	$[11, 22]$
12	$[-X, -X, Y]$	$[\frac{1}{2}, \frac{1}{2}, x]$	$[12, 24]$

Table 39: Wyckoff bond: 12d@6g

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

continued ...

Table 39

No.	vector	center	mapping
4	$[Y, 0, -X]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	[6, -7]
5	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, x]$	[9, -12]
6	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	[10, -11]
7	$[X, 0, Y]$	$[\frac{1}{2}, x, \frac{1}{2}]$	[13, -16]
8	$[-X, 0, Y]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	[14, -15]
9	$[0, Y, X]$	$[x, \frac{1}{2}, \frac{1}{2}]$	[17, -20]
10	$[0, Y, -X]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	[18, -19]
11	$[Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, x]$	[21, -24]
12	$[Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	[22, -23]

Table 40: Wyckoff bond: 24e06g

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, \frac{1}{2}, \frac{1}{2}]$	[1]
2	$[-X, -Y, Z]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	[2]
3	$[-X, Y, -Z]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	[3]
4	$[X, -Y, -Z]$	$[x, \frac{1}{2}, \frac{1}{2}]$	[4]
5	$[Z, X, Y]$	$[\frac{1}{2}, x, \frac{1}{2}]$	[5]
6	$[Z, -X, -Y]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	[6]
7	$[-Z, -X, Y]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	[7]
8	$[-Z, X, -Y]$	$[\frac{1}{2}, x, \frac{1}{2}]$	[8]
9	$[Y, Z, X]$	$[\frac{1}{2}, \frac{1}{2}, x]$	[9]
10	$[-Y, Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	[10]
11	$[Y, -Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{2}, \frac{1}{2}, x]$	[12]
13	$[Y, X, Z]$	$[\frac{1}{2}, x, \frac{1}{2}]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	[14]
15	$[Y, -X, -Z]$	$[\frac{1}{2}, -x, \frac{1}{2}]$	[15]
16	$[-Y, X, -Z]$	$[\frac{1}{2}, x, \frac{1}{2}]$	[16]
17	$[X, Z, Y]$	$[x, \frac{1}{2}, \frac{1}{2}]$	[17]
18	$[-X, Z, -Y]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	[18]
19	$[-X, -Z, Y]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	[19]
20	$[X, -Z, -Y]$	$[x, \frac{1}{2}, \frac{1}{2}]$	[20]
21	$[Z, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, x]$	[21]
22	$[Z, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	[22]
23	$[-Z, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, -x]$	[23]
24	$[-Z, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, x]$	[24]

\* Wyckoff site: 12h, site symmetry: 2..

Table 41: Wyckoff bond: 12a@12h

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, \frac{1}{2}, 0]$	$[1, -4]$
2	$[0, -X, Y]$	$[-x, \frac{1}{2}, 0]$	$[2, -3]$
3	$[Y, 0, X]$	$[0, x, \frac{1}{2}]$	$[5, -8]$
4	$[Y, 0, -X]$	$[0, -x, \frac{1}{2}]$	$[6, -7]$
5	$[X, Y, 0]$	$[\frac{1}{2}, 0, x]$	$[9, -12]$
6	$[-X, Y, 0]$	$[\frac{1}{2}, 0, -x]$	$[10, -11]$
7	$[X, 0, Y]$	$[\frac{1}{2}, x, 0]$	$[13, -16]$
8	$[-X, 0, Y]$	$[\frac{1}{2}, -x, 0]$	$[14, -15]$
9	$[0, Y, X]$	$[x, 0, \frac{1}{2}]$	$[17, -20]$
10	$[0, Y, -X]$	$[-x, 0, \frac{1}{2}]$	$[18, -19]$
11	$[Y, X, 0]$	$[0, \frac{1}{2}, x]$	$[21, -24]$
12	$[Y, -X, 0]$	$[0, \frac{1}{2}, -x]$	$[22, -23]$

Table 42: Wyckoff bond: 12b@12h

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, \frac{1}{2}, 0]$	$[1, 4]$
2	$[-X, 0, 0]$	$[-x, \frac{1}{2}, 0]$	$[2, 3]$
3	$[0, X, 0]$	$[0, x, \frac{1}{2}]$	$[5, 8]$
4	$[0, -X, 0]$	$[0, -x, \frac{1}{2}]$	$[6, 7]$
5	$[0, 0, X]$	$[\frac{1}{2}, 0, x]$	$[9, 12]$
6	$[0, 0, -X]$	$[\frac{1}{2}, 0, -x]$	$[10, 11]$
7	$[0, X, 0]$	$[\frac{1}{2}, x, 0]$	$[13, 16]$
8	$[0, -X, 0]$	$[\frac{1}{2}, -x, 0]$	$[14, 15]$
9	$[X, 0, 0]$	$[x, 0, \frac{1}{2}]$	$[17, 20]$
10	$[-X, 0, 0]$	$[-x, 0, \frac{1}{2}]$	$[18, 19]$
11	$[0, 0, X]$	$[0, \frac{1}{2}, x]$	$[21, 24]$
12	$[0, 0, -X]$	$[0, \frac{1}{2}, -x]$	$[22, 23]$

Table 43: Wyckoff bond: 24c@12h

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

continued ...



Table 43

No.	vector	center	mapping
10	$[-Y, Z, -X]$	$[\frac{1}{2}, 0, -x]$	[10]
11	$[Y, -Z, -X]$	$[\frac{1}{2}, 0, -x]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{2}, 0, x]$	[12]
13	$[Y, X, Z]$	$[\frac{1}{2}, x, 0]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{2}, -x, 0]$	[14]
15	$[Y, -X, -Z]$	$[\frac{1}{2}, -x, 0]$	[15]
16	$[-Y, X, -Z]$	$[\frac{1}{2}, x, 0]$	[16]
17	$[X, Z, Y]$	$[x, 0, \frac{1}{2}]$	[17]
18	$[-X, Z, -Y]$	$[-x, 0, \frac{1}{2}]$	[18]
19	$[-X, -Z, Y]$	$[-x, 0, \frac{1}{2}]$	[19]
20	$[X, -Z, -Y]$	$[x, 0, \frac{1}{2}]$	[20]
21	$[Z, Y, X]$	$[0, \frac{1}{2}, x]$	[21]
22	$[Z, -Y, -X]$	$[0, \frac{1}{2}, -x]$	[22]
23	$[-Z, Y, -X]$	$[0, \frac{1}{2}, -x]$	[23]
24	$[-Z, -Y, X]$	$[0, \frac{1}{2}, x]$	[24]

\* Wyckoff site: 12i, site symmetry:  $\bar{3}m$

Table 44: Wyckoff bond: 12a@12i

No.	vector	center	mapping
1	$[X, X, Y]$	$[x, x, z]$	[1,13]
2	$[-X, -X, Y]$	$[-x, -x, z]$	[2,14]
3	$[-X, X, -Y]$	$[-x, x, -z]$	[3,16]
4	$[X, -X, -Y]$	$[x, -x, -z]$	[4,15]
5	$[Y, X, X]$	$[z, x, x]$	[5,21]
6	$[Y, -X, -X]$	$[z, -x, -x]$	[6,22]
7	$[-Y, -X, X]$	$[-z, -x, x]$	[7,24]
8	$[-Y, X, -X]$	$[-z, x, -x]$	[8,23]
9	$[X, Y, X]$	$[x, z, x]$	[9,17]
10	$[-X, Y, -X]$	$[-x, z, -x]$	[10,18]
11	$[X, -Y, -X]$	$[x, -z, -x]$	[11,20]
12	$[-X, -Y, X]$	$[-x, -z, x]$	[12,19]

Table 45: Wyckoff bond: 12b@12i

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, z]$	[1,-13]
2	$[-X, X, 0]$	$[-x, -x, z]$	[2,-14]
3	$[-X, -X, 0]$	$[-x, x, -z]$	[3,-16]
4	$[X, X, 0]$	$[x, -x, -z]$	[4,-15]
5	$[0, X, -X]$	$[z, x, x]$	[5,-21]

*continued ...*

Table 45

No.	vector	center	mapping
6	$[0, -X, X]$	$[z, -x, -x]$	$[6, -22]$
7	$[0, -X, -X]$	$[-z, -x, x]$	$[7, -24]$
8	$[0, X, X]$	$[-z, x, -x]$	$[8, -23]$
9	$[-X, 0, X]$	$[x, z, x]$	$[9, -17]$
10	$[X, 0, -X]$	$[-x, z, -x]$	$[10, -18]$
11	$[-X, 0, -X]$	$[x, -z, -x]$	$[11, -20]$
12	$[X, 0, X]$	$[-x, -z, x]$	$[12, -19]$

Table 46: Wyckoff bond: 24c@12i

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -x, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, x, -z]$	[3]
4	$[X, -Y, -Z]$	$[x, -x, -z]$	[4]
5	$[Z, X, Y]$	$[z, x, x]$	[5]
6	$[Z, -X, -Y]$	$[z, -x, -x]$	[6]
7	$[-Z, -X, Y]$	$[-z, -x, x]$	[7]
8	$[-Z, X, -Y]$	$[-z, x, -x]$	[8]
9	$[Y, Z, X]$	$[x, z, x]$	[9]
10	$[-Y, Z, -X]$	$[-x, z, -x]$	[10]
11	$[Y, -Z, -X]$	$[x, -z, -x]$	[11]
12	$[-Y, -Z, X]$	$[-x, -z, x]$	[12]
13	$[Y, X, Z]$	$[x, x, z]$	[13]
14	$[-Y, -X, Z]$	$[-x, -x, z]$	[14]
15	$[Y, -X, -Z]$	$[x, -x, -z]$	[15]
16	$[-Y, X, -Z]$	$[-x, x, -z]$	[16]
17	$[X, Z, Y]$	$[x, z, x]$	[17]
18	$[-X, Z, -Y]$	$[-x, z, -x]$	[18]
19	$[-X, -Z, Y]$	$[-x, -z, x]$	[19]
20	$[X, -Z, -Y]$	$[x, -z, -x]$	[20]
21	$[Z, Y, X]$	$[z, x, x]$	[21]
22	$[Z, -Y, -X]$	$[z, -x, -x]$	[22]
23	$[-Z, Y, -X]$	$[-z, x, -x]$	[23]
24	$[-Z, -Y, X]$	$[-z, -x, x]$	[24]

\* Wyckoff site: 24j, site symmetry: 1

Table 47: Wyckoff bond: 24a@24j

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]

*continued ...*

Table 47

No.	vector	center	mapping
2	$[-X, -Y, Z]$	$[-x, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, -z]$	[4]
5	$[Z, X, Y]$	$[z, x, y]$	[5]
6	$[Z, -X, -Y]$	$[z, -x, -y]$	[6]
7	$[-Z, -X, Y]$	$[-z, -x, y]$	[7]
8	$[-Z, X, -Y]$	$[-z, x, -y]$	[8]
9	$[Y, Z, X]$	$[y, z, x]$	[9]
10	$[-Y, Z, -X]$	$[-y, z, -x]$	[10]
11	$[Y, -Z, -X]$	$[y, -z, -x]$	[11]
12	$[-Y, -Z, X]$	$[-y, -z, x]$	[12]
13	$[Y, X, Z]$	$[y, x, z]$	[13]
14	$[-Y, -X, Z]$	$[-y, -x, z]$	[14]
15	$[Y, -X, -Z]$	$[y, -x, -z]$	[15]
16	$[-Y, X, -Z]$	$[-y, x, -z]$	[16]
17	$[X, Z, Y]$	$[x, z, y]$	[17]
18	$[-X, Z, -Y]$	$[-x, z, -y]$	[18]
19	$[-X, -Z, Y]$	$[-x, -z, y]$	[19]
20	$[X, -Z, -Y]$	$[x, -z, -y]$	[20]
21	$[Z, Y, X]$	$[z, y, x]$	[21]
22	$[Z, -Y, -X]$	$[z, -y, -x]$	[22]
23	$[-Z, Y, -X]$	$[-z, y, -x]$	[23]
24	$[-Z, -Y, X]$	$[-z, -y, x]$	[24]