

SG No. 216 T_d^2 $F\bar{4}3m$ [cubic]

* plus set: $+ [0, 0, 0]$, $+ [0, \frac{1}{2}, \frac{1}{2}]$, $+ [\frac{1}{2}, 0, \frac{1}{2}]$, $+ [\frac{1}{2}, \frac{1}{2}, 0]$

* Wyckoff site: **4a**, site symmetry: $-43\bar{m}$

Table 1: Wyckoff bond: 12a@4a

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: 16b@4a

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: 24c@4a

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: 48d@4a

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: **48e@4a**

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: **96f@4a**

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: **4b**, site symmetry: **-43m**

Table 7: Wyckoff bond: **12a@4b**

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: **16b@4b**

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: **24c@4b**

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: **48d@4b**

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: **48e@4b**

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: **96f@4b**

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: 4c, site symmetry: $\bar{4}3m$

Table 13: Wyckoff bond: 12a@4c

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

Table 14: Wyckoff bond: 16b@4c

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

Table 15: Wyckoff bond: 24c@4c

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

Table 16: Wyckoff bond: 48d@4c

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

Table 17: Wyckoff bond: 48e@4c

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

Table 18: Wyckoff bond: 96f@4c

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

continued ...

Table 18

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

* Wyckoff site: 4d, site symmetry: $\bar{4}3m$

Table 19: Wyckoff bond: 12a@4d

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

Table 20: Wyckoff bond: 16b@4d

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

Table 21: Wyckoff bond: 24c@4d

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

continued ...

Table 21

No.	vector	center	mapping
5	$[X, 0, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[9, -10, 17, -18]$
6	$[X, 0, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[11, -12, -19, 20]$

Table 22: Wyckoff bond: 48d@4d

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

Table 23: Wyckoff bond: 48e@4d

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

Table 24: Wyckoff bond: 96f@4d

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

continued ...

Table 24

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

* Wyckoff site: 16e, site symmetry: .3m

Table 25: Wyckoff bond: 16a@16e

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 26: Wyckoff bond: 48b@16e

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]

continued ...

Table 26

No.	vector	center	mapping
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 27: Wyckoff bond: **48c@16e**

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 28: Wyckoff bond: **96d@16e**

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	$[Y, -X, -Z]$	$[x, -x, -x]$	$[15]$

continued ...

Table 28

No.	vector	center	mapping
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: 24f, site symmetry: $2.mm$

Table 29: Wyckoff bond: 24a@24f

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 30: Wyckoff bond: 24b@24f

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 31: Wyckoff bond: 48c@24f

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]

continued ...

Table 31

No.	vector	center	mapping
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 32: Wyckoff bond: **48d@24f**

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, 0, 0]$	$[1, -4]$
2	$[0, -X, Y]$	$[-x, 0, 0]$	$[2, -3]$
3	$[Y, 0, X]$	$[0, x, 0]$	$[5, -8]$
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 33: Wyckoff bond: **96e@24f**

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	$[Y, -X, -Z]$	$[0, -x, 0]$	$[15]$

continued ...

Table 33

No.	vector	center	mapping
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: 24g, site symmetry: 2.mm

Table 34: Wyckoff bond: 24a@24g

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

Table 35: Wyckoff bond: 24b@24g

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

Table 36: Wyckoff bond: 48c@24g

No.	vector	center	mapping
1	$[Y, X, X]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[1, 17]
2	$[-Y, -X, X]$	$[-x, \frac{3}{4}, \frac{1}{4}]$	[2, 19]
3	$[-Y, X, -X]$	$[-x, \frac{3}{4}, \frac{1}{4}]$	[3, 18]
4	$[Y, -X, -X]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[4, 20]
5	$[X, Y, X]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[5, 13]

continued ...

Table 36

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

Table 37: Wyckoff bond: 48d@24g

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

Table 38: Wyckoff bond: 96e@24g

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

continued ...

Table 38

No.	vector	center	mapping
16	$[-Y, X, -Z]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[16]
17	$[X, Z, Y]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[17]
18	$[-X, Z, -Y]$	$[-x, \frac{3}{4}, \frac{1}{4}]$	[18]
19	$[-X, -Z, Y]$	$[-x, \frac{3}{4}, \frac{1}{4}]$	[19]
20	$[X, -Z, -Y]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[20]
21	$[Z, Y, X]$	$[\frac{1}{4}, \frac{1}{4}, x]$	[21]
22	$[Z, -Y, -X]$	$[\frac{3}{4}, \frac{1}{4}, -x]$	[22]
23	$[-Z, Y, -X]$	$[\frac{3}{4}, \frac{1}{4}, -x]$	[23]
24	$[-Z, -Y, X]$	$[\frac{1}{4}, \frac{1}{4}, x]$	[24]

* Wyckoff site: 48h, site symmetry: $\bar{3}m$

Table 39: Wyckoff bond: 48a@48h

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 40: Wyckoff bond: 48b@48h

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]
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]

continued ...

Table 40

No.	vector	center	mapping
12	$[X, 0, X]$	$[-x, -z, x]$	$[12, -19]$

Table 41: Wyckoff bond: 96c@48h

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: 96i, site symmetry: 1

Table 42: Wyckoff bond: 96a@96i

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

continued ...

Table 42

No.	vector	center	mapping
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]