

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: 12f@3d

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: 24g@3d

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: 24e@6f

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: 24e@6g

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: . . 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]