

SG No. 208 O^2 $P4_232$ [cubic]

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

* Wyckoff site: 2a, site symmetry: 23.

Table 1: Wyckoff bond: 6a@2a

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

Table 2: Wyckoff bond: 8b@2a

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

Table 3: Wyckoff bond: 12c@2a

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]	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[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 4: Wyckoff bond: 24d@2a

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	$[Y, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[13]
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: 4b, site symmetry: .32

Table 5: Wyckoff bond: 4a@4b

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

Table 6: Wyckoff bond: 12b@4b

No.	vector	center	mapping
1	$[X, X, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1, -14]
2	$[-X, -X, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[2, -13]
3	$[-X, X, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[3, -15]
4	$[X, -X, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[4, -16]

continued ...

Table 6

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

Table 7: Wyckoff bond: 12c@4b

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

Table 8: Wyckoff bond: 24d@4b

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

continued ...

Table 8

No.	vector	center	mapping
15	[Y, -X, Z]	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[15]
16	[-Y, X, Z]	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[16]
17	[X, Z, -Y]	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[17]
18	[-X, Z, Y]	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[18]
19	[-X, -Z, -Y]	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[19]
20	[X, -Z, Y]	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[20]
21	[Z, Y, -X]	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[21]
22	[Z, -Y, X]	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[22]
23	[-Z, Y, X]	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[23]
24	[-Z, -Y, -X]	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[24]

* Wyckoff site: 4c, site symmetry: .32

Table 9: Wyckoff bond: 4a@4c

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

Table 10: Wyckoff bond: 12b@4c

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

Table 11: Wyckoff bond: 12c@4c

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

Table 12: Wyckoff bond: 24d@4c

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

* Wyckoff site: 6d, site symmetry: 222..

Table 13: Wyckoff bond: 6a@6d

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

Table 14: Wyckoff bond: 6b@6d

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	$[0, 0, -X]$	$[0, \frac{1}{2}, 0]$	$[13, 14, -15, -16]$
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 15: Wyckoff bond: 6c@6d

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

Table 16: Wyckoff bond: 12d@6d

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	$[Y, X, 0]$	$[0, \frac{1}{2}, 0]$	$[13, -14]$
8	$[Y, -X, 0]$	$[0, \frac{1}{2}, 0]$	$[15, -16]$
9	$[X, 0, -Y]$	$[\frac{1}{2}, 0, 0]$	$[17, -18]$

continued ...

Table 16

No.	vector	center	mapping
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 17: Wyckoff bond: 12e@6d

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

Table 18: Wyckoff bond: 12f@6d

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	$[X, 0, -Y]$	$[0, \frac{1}{2}, 0]$	[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 19: Wyckoff bond: 24g@6d

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	$[Y, X, -Z]$	$[0, \frac{1}{2}, 0]$	[13]
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: 6e, site symmetry: 2.22

Table 20: Wyckoff bond: 6a@6e

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

Table 21: Wyckoff bond: 6b@6e

No.	vector	center	mapping
1	$[0, X, -X]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[1,-4,-18,19]
2	$[0, -X, -X]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[2,-3,17,-20]

continued ...

Table 21

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

Table 22: Wyckoff bond: 6c@6e

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

Table 23: Wyckoff bond: 12d@6e

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

Table 24: Wyckoff bond: 12e@6e

No.	vector	center	mapping
1	$[Y, X, -X]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[1, -18]
2	$[-Y, -X, -X]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[2, -20]
3	$[-Y, X, X]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[3, -17]
4	$[Y, -X, X]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[4, -19]
5	$[-X, Y, X]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[5, -15]

continued ...

Table 24

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

Table 25: Wyckoff bond: 12f@6e

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

Table 26: Wyckoff bond: 24g@6e

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

continued ...

Table 26

No.	vector	center	mapping
16	$[-Y, X, Z]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[16]
17	$[X, Z, -Y]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[19]
20	$[X, -Z, Y]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[20]
21	$[Z, Y, -X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[21]
22	$[Z, -Y, X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[22]
23	$[-Z, Y, X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[24]

* Wyckoff site: 6f, site symmetry: 2.22

Table 27: Wyckoff bond: 6a@6f

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

Table 28: Wyckoff bond: 6b@6f

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

Table 29: Wyckoff bond: 6c@6f

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

continued ...

Table 29

No.	vector	center	mapping
6	[0, 0, -X]	$[\frac{1}{2}, 0, \frac{3}{4}]$	[10, 11, -22, -23]

Table 30: Wyckoff bond: 12d@6f

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

Table 31: Wyckoff bond: 12e@6f

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

Table 32: Wyckoff bond: 12f@6f

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

continued ...

Table 32

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

Table 33: Wyckoff bond: 24g@6f

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

* Wyckoff site: 8g, site symmetry: .3.

Table 34: Wyckoff bond: 8a@8g

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

Table 35: Wyckoff bond: 24b@8g

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 + 1/2, x + 1/2, 1/2 - x]	[13]
14	[-Y, -X, -Z]	[1/2 - x, 1/2 - x, 1/2 - x]	[14]
15	[Y, -X, Z]	[x + 1/2, 1/2 - x, x + 1/2]	[15]
16	[-Y, X, Z]	[1/2 - x, x + 1/2, x + 1/2]	[16]
17	[X, Z, -Y]	[x + 1/2, x + 1/2, 1/2 - x]	[17]
18	[-X, Z, Y]	[1/2 - x, x + 1/2, x + 1/2]	[18]
19	[-X, -Z, -Y]	[1/2 - x, 1/2 - x, 1/2 - x]	[19]
20	[X, -Z, Y]	[x + 1/2, 1/2 - x, x + 1/2]	[20]
21	[Z, Y, -X]	[x + 1/2, x + 1/2, 1/2 - x]	[21]
22	[Z, -Y, X]	[x + 1/2, 1/2 - x, x + 1/2]	[22]
23	[-Z, Y, X]	[1/2 - x, x + 1/2, x + 1/2]	[23]
24	[-Z, -Y, -X]	[1/2 - x, 1/2 - x, 1/2 - x]	[24]

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

Table 36: Wyckoff bond: 12a@12h

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]	[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]	[13, -16]
8	[-X, 0, -Y]	[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[14, -15]
9	[0, Y, -X]	[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[17, -20]
10	[0, Y, X]	[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]	[18, -19]
11	[Y, X, 0]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]	[21, -24]
12	[Y, -X, 0]	[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]	[22, -23]

Table 37: Wyckoff bond: 12b@12h

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

Table 38: Wyckoff bond: 24c@12h

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]

continued ...

Table 38

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

* Wyckoff site: 12i, site symmetry: 2..

Table 39: Wyckoff bond: 12a@12i

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

Table 40: Wyckoff bond: 12b@12i

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

continued ...

Table 40

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

Table 41: Wyckoff bond: 24c@12i

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

* Wyckoff site: 12j, site symmetry: 2..

Table 42: Wyckoff bond: 12a@12j

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

continued ...

Table 42

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

Table 43: Wyckoff bond: 12b@12j

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	$[0, X, 0]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[13,16]
8	$[0, -X, 0]$	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[14,15]
9	$[X, 0, 0]$	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[17,20]
10	$[-X, 0, 0]$	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[18,19]
11	$[0, 0, -X]$	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[21,24]
12	$[0, 0, X]$	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[22,23]

Table 44: Wyckoff bond: 24c@12j

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]
10	$[-Y, Z, -X]$	$[\frac{1}{2}, 0, -x]$	[10]
11	$[Y, -Z, -X]$	$[\frac{1}{2}, 0, -x]$	[11]

continued ...

Table 44

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

* Wyckoff site: 12k, site symmetry: ..2

Table 45: Wyckoff bond: 12a@12k

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

Table 46: Wyckoff bond: 12b@12k

No.	vector	center	mapping
1	$[0, X, -X]$	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[1,19]
2	$[0, -X, -X]$	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[2,17]
3	$[0, X, X]$	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[3,20]
4	$[0, -X, X]$	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[4,18]
5	$[-X, 0, X]$	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[5,14]
6	$[-X, 0, -X]$	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[6,16]
7	$[X, 0, X]$	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[7,13]

continued ...

Table 46

No.	vector	center	mapping
8	$[X, 0, -X]$	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[8,15]
9	$[X, -X, 0]$	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[9,24]
10	$[-X, -X, 0]$	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[10,22]
11	$[X, X, 0]$	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[11,23]
12	$[-X, X, 0]$	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[12,21]

Table 47: Wyckoff bond: 24c@12k

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

* Wyckoff site: 12l, site symmetry: ..2

Table 48: Wyckoff bond: 12a@12l

No.	vector	center	mapping
1	$[Y, X, -X]$	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[1,-18]
2	$[-Y, -X, -X]$	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[2,-20]
3	$[-Y, X, X]$	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[3,-17]

continued ...

Table 48

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

Table 49: Wyckoff bond: 12b@121

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

Table 50: Wyckoff bond: 24c@121

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

continued ...

Table 50

No.	vector	center	mapping
14	$[-Y, -X, -Z]$	$[\frac{1}{2} - y, \frac{1}{4}, -y]$	[14]
15	$[Y, -X, Z]$	$[y + \frac{1}{2}, \frac{1}{4}, y]$	[15]
16	$[-Y, X, Z]$	$[\frac{1}{2} - y, \frac{3}{4}, y]$	[16]
17	$[X, Z, -Y]$	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{4}, -y, \frac{1}{2} - y]$	[19]
20	$[X, -Z, Y]$	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[20]
21	$[Z, Y, -X]$	$[y, y + \frac{1}{2}, \frac{1}{4}]$	[21]
22	$[Z, -Y, X]$	$[y, \frac{1}{2} - y, \frac{3}{4}]$	[22]
23	$[-Z, Y, X]$	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	[24]

* Wyckoff site: 24m, site symmetry: 1

Table 51: Wyckoff bond: 24a@24m

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]
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	$[Y, X, -Z]$	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[14]
15	$[Y, -X, Z]$	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[15]
16	$[-Y, X, Z]$	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[16]
17	$[X, Z, -Y]$	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[19]
20	$[X, -Z, Y]$	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[20]
21	$[Z, Y, -X]$	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[21]
22	$[Z, -Y, X]$	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[24]