

SG No. 223 O_h^3 $Pm\bar{3}n$ [cubic]

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

* Wyckoff site: 2a, site symmetry: m-3.

Table 1: Wyckoff bond: 6a@2a

No.	vector	center	mapping
1	[X, 0, 0]	[0, 0, 0]	[1, -2, -3, 4, -25, 26, 27, -28]
2	[0, X, 0]	[0, 0, 0]	[5, -6, -7, 8, -29, 30, 31, -32]
3	[0, 0, X]	[0, 0, 0]	[9, -10, -11, 12, -33, 34, 35, -36]
4	[0, X, 0]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[13, -14, -15, 16, -37, 38, 39, -40]
5	[X, 0, 0]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[17, -18, -19, 20, -41, 42, 43, -44]
6	[0, 0, -X]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[21, -22, -23, 24, -45, 46, 47, -48]

Table 2: Wyckoff bond: 8b@2a

No.	vector	center	mapping
1	[X, X, X]	[0, 0, 0]	[1, 5, 9, -25, -29, -33]
2	[-X, -X, X]	[0, 0, 0]	[2, 7, 12, -26, -31, -36]
3	[-X, X, -X]	[0, 0, 0]	[3, 8, 10, -27, -32, -34]
4	[X, -X, -X]	[0, 0, 0]	[4, 6, 11, -28, -30, -35]
5	[X, X, -X]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[13, 17, 21, -37, -41, -45]
6	[-X, -X, -X]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[14, 19, 24, -38, -43, -48]
7	[X, -X, X]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[15, 20, 22, -39, -44, -46]
8	[-X, X, X]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[16, 18, 23, -40, -42, -47]

Table 3: Wyckoff bond: 12c@2a

No.	vector	center	mapping
1	[X, Y, 0]	[0, 0, 0]	[1, -2, -25, 26]
2	[-X, Y, 0]	[0, 0, 0]	[3, -4, -27, 28]
3	[0, X, Y]	[0, 0, 0]	[5, -6, -29, 30]
4	[0, -X, Y]	[0, 0, 0]	[7, -8, -31, 32]
5	[Y, 0, X]	[0, 0, 0]	[9, -10, -33, 34]
6	[Y, 0, -X]	[0, 0, 0]	[11, -12, -35, 36]
7	[Y, X, 0]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[13, -14, -37, 38]
8	[Y, -X, 0]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[15, -16, -39, 40]
9	[X, 0, -Y]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[17, -18, -41, 42]
10	[-X, 0, -Y]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[19, -20, -43, 44]
11	[0, Y, -X]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[21, -22, -45, 46]
12	[0, Y, X]	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[23, -24, -47, 48]

Table 4: Wyckoff bond: 24d@2a

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -25]$
2	$[-X, -Y, Z]$	$[0, 0, 0]$	$[2, -26]$
3	$[-X, Y, -Z]$	$[0, 0, 0]$	$[3, -27]$
4	$[X, -Y, -Z]$	$[0, 0, 0]$	$[4, -28]$
5	$[Z, X, Y]$	$[0, 0, 0]$	$[5, -29]$
6	$[Z, -X, -Y]$	$[0, 0, 0]$	$[6, -30]$
7	$[-Z, -X, Y]$	$[0, 0, 0]$	$[7, -31]$
8	$[-Z, X, -Y]$	$[0, 0, 0]$	$[8, -32]$
9	$[Y, Z, X]$	$[0, 0, 0]$	$[9, -33]$
10	$[-Y, Z, -X]$	$[0, 0, 0]$	$[10, -34]$
11	$[Y, -Z, -X]$	$[0, 0, 0]$	$[11, -35]$
12	$[-Y, -Z, X]$	$[0, 0, 0]$	$[12, -36]$
13	$[Y, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[13, -37]$
14	$[-Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[14, -38]$
15	$[Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[15, -39]$
16	$[-Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[16, -40]$
17	$[X, Z, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[17, -41]$
18	$[-X, Z, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[18, -42]$
19	$[-X, -Z, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[19, -43]$
20	$[X, -Z, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[20, -44]$
21	$[Z, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[21, -45]$
22	$[Z, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[22, -46]$
23	$[-Z, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[23, -47]$
24	$[-Z, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[24, -48]$

* Wyckoff site: 6b, site symmetry: mmm..

Table 5: Wyckoff bond: 6a@6b

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -3, 4, -25, 26, 27, -28]$
2	$[0, X, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6, -7, 8, -29, 30, 31, -32]$
3	$[0, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -10, -11, 12, -33, 34, 35, -36]$
4	$[0, X, 0]$	$[0, \frac{1}{2}, 0]$	$[13, -14, -15, 16, -37, 38, 39, -40]$
5	$[X, 0, 0]$	$[\frac{1}{2}, 0, 0]$	$[17, -18, -19, 20, -41, 42, 43, -44]$
6	$[0, 0, -X]$	$[0, 0, \frac{1}{2}]$	$[21, -22, -23, 24, -45, 46, 47, -48]$

Table 6: Wyckoff bond: 6b@6b

No.	vector	center	mapping
1	$[0, 0, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, -3, -4, -25, -26, 27, 28]$
2	$[X, 0, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, 6, -7, -8, -29, -30, 31, 32]$

continued ...

Table 6

No.	vector	center	mapping
3	$[0, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, 10, -11, -12, -33, -34, 35, 36]$
4	$[0, 0, -X]$	$[0, \frac{1}{2}, 0]$	$[13, 14, -15, -16, -37, -38, 39, 40]$
5	$[0, X, 0]$	$[\frac{1}{2}, 0, 0]$	$[17, 18, -19, -20, -41, -42, 43, 44]$
6	$[X, 0, 0]$	$[0, 0, \frac{1}{2}]$	$[21, 22, -23, -24, -45, -46, 47, 48]$

Table 7: Wyckoff bond: 6c@6b

No.	vector	center	mapping
1	$[0, X, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, 3, -4, -25, 26, -27, 28]$
2	$[0, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6, 7, -8, -29, 30, -31, 32]$
3	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -10, 11, -12, -33, 34, -35, 36]$
4	$[X, 0, 0]$	$[0, \frac{1}{2}, 0]$	$[13, -14, 15, -16, -37, 38, -39, 40]$
5	$[0, 0, -X]$	$[\frac{1}{2}, 0, 0]$	$[17, -18, 19, -20, -41, 42, -43, 44]$
6	$[0, X, 0]$	$[0, 0, \frac{1}{2}]$	$[21, -22, 23, -24, -45, 46, -47, 48]$

Table 8: Wyckoff bond: 12d@6b

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -25, 26]$
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -4, -27, 28]$
3	$[0, X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -6, -29, 30]$
4	$[0, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[7, -8, -31, 32]$
5	$[Y, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -10, -33, 34]$
6	$[Y, 0, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[11, -12, -35, 36]$
7	$[Y, X, 0]$	$[0, \frac{1}{2}, 0]$	$[13, -14, -37, 38]$
8	$[Y, -X, 0]$	$[0, \frac{1}{2}, 0]$	$[15, -16, -39, 40]$
9	$[X, 0, -Y]$	$[\frac{1}{2}, 0, 0]$	$[17, -18, -41, 42]$
10	$[-X, 0, -Y]$	$[\frac{1}{2}, 0, 0]$	$[19, -20, -43, 44]$
11	$[0, Y, -X]$	$[0, 0, \frac{1}{2}]$	$[21, -22, -45, 46]$
12	$[0, Y, X]$	$[0, 0, \frac{1}{2}]$	$[23, -24, -47, 48]$

Table 9: Wyckoff bond: 12e@6b

No.	vector	center	mapping
1	$[Y, 0, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -3, -25, 27]$
2	$[-Y, 0, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -4, -26, 28]$
3	$[X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -7, -29, 31]$
4	$[X, -Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, -8, -30, 32]$
5	$[0, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -11, -33, 35]$

continued ...

Table 9

No.	vector	center	mapping
6	$[0, X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[10, -12, -34, 36]$
7	$[0, Y, -X]$	$[0, \frac{1}{2}, 0]$	$[13, -15, -37, 39]$
8	$[0, -Y, -X]$	$[0, \frac{1}{2}, 0]$	$[14, -16, -38, 40]$
9	$[Y, X, 0]$	$[\frac{1}{2}, 0, 0]$	$[17, -19, -41, 43]$
10	$[-Y, X, 0]$	$[\frac{1}{2}, 0, 0]$	$[18, -20, -42, 44]$
11	$[X, 0, -Y]$	$[0, 0, \frac{1}{2}]$	$[21, -23, -45, 47]$
12	$[X, 0, Y]$	$[0, 0, \frac{1}{2}]$	$[22, -24, -46, 48]$

Table 10: Wyckoff bond: 12f@6b

No.	vector	center	mapping
1	$[0, X, Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -4, -25, 28]$
2	$[0, -X, Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -3, -26, 27]$
3	$[Y, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -8, -29, 32]$
4	$[Y, 0, -X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, -7, -30, 31]$
5	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -12, -33, 36]$
6	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[10, -11, -34, 35]$
7	$[X, 0, -Y]$	$[0, \frac{1}{2}, 0]$	$[13, -16, -37, 40]$
8	$[-X, 0, -Y]$	$[0, \frac{1}{2}, 0]$	$[14, -15, -38, 39]$
9	$[0, Y, -X]$	$[\frac{1}{2}, 0, 0]$	$[17, -20, -41, 44]$
10	$[0, Y, X]$	$[\frac{1}{2}, 0, 0]$	$[18, -19, -42, 43]$
11	$[Y, X, 0]$	$[0, 0, \frac{1}{2}]$	$[21, -24, -45, 48]$
12	$[Y, -X, 0]$	$[0, 0, \frac{1}{2}]$	$[22, -23, -46, 47]$

Table 11: Wyckoff bond: 24g@6b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -25]$
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -26]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -27]$
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[4, -28]$
5	$[Z, X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, -29]$
6	$[Z, -X, -Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[6, -30]$
7	$[-Z, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[7, -31]$
8	$[-Z, X, -Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[8, -32]$
9	$[Y, Z, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[9, -33]$
10	$[-Y, Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[10, -34]$
11	$[Y, -Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[11, -35]$
12	$[-Y, -Z, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[12, -36]$
13	$[Y, X, -Z]$	$[0, \frac{1}{2}, 0]$	$[13, -37]$
14	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, 0]$	$[14, -38]$
15	$[Y, -X, Z]$	$[0, \frac{1}{2}, 0]$	$[15, -39]$

continued ...

Table 11

No.	vector	center	mapping
16	$[-Y, X, Z]$	$[0, \frac{1}{2}, 0]$	[16, -40]
17	$[X, Z, -Y]$	$[\frac{1}{2}, 0, 0]$	[17, -41]
18	$[-X, Z, Y]$	$[\frac{1}{2}, 0, 0]$	[18, -42]
19	$[-X, -Z, -Y]$	$[\frac{1}{2}, 0, 0]$	[19, -43]
20	$[X, -Z, Y]$	$[\frac{1}{2}, 0, 0]$	[20, -44]
21	$[Z, Y, -X]$	$[0, 0, \frac{1}{2}]$	[21, -45]
22	$[Z, -Y, X]$	$[0, 0, \frac{1}{2}]$	[22, -46]
23	$[-Z, Y, X]$	$[0, 0, \frac{1}{2}]$	[23, -47]
24	$[-Z, -Y, -X]$	$[0, 0, \frac{1}{2}]$	[24, -48]

* Wyckoff site: 6c, site symmetry: $-4\bar{m}.2$

Table 12: Wyckoff bond: 6a@6c

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[1, 4, -18, -19, 26, 27, -41, -44]
2	$[-X, 0, 0]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[2, 3, -17, -20, 25, 28, -42, -43]
3	$[0, X, 0]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[5, 8, -14, -15, 30, 31, -37, -40]
4	$[0, -X, 0]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[6, 7, -13, -16, 29, 32, -38, -39]
5	$[0, 0, X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[9, 12, -21, -24, 34, 35, -46, -47]
6	$[0, 0, -X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[10, 11, -22, -23, 33, 36, -45, -48]

Table 13: Wyckoff bond: 12b@6c

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]
7	$[0, -X, -X]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[25, -28, 42, -43]
8	$[0, X, -X]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[26, -27, -41, 44]
9	$[-X, 0, -X]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[29, -32, -38, 39]
10	$[-X, 0, X]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[30, -31, 37, -40]
11	$[-X, -X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[33, -36, 45, -48]
12	$[X, -X, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[34, -35, -46, 47]

Table 14: Wyckoff bond: 12c@6c

No.	vector	center	mapping
1	$[0, 0, X]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	$[1, -4, -26, 27]$
2	$[0, 0, X]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	$[2, -3, -25, 28]$
3	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	$[5, -8, -30, 31]$
4	$[X, 0, 0]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	$[6, -7, -29, 32]$
5	$[0, X, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[9, -12, -34, 35]$
6	$[0, X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[10, -11, -33, 36]$
7	$[0, 0, -X]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	$[13, -16, -38, 39]$
8	$[0, 0, -X]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	$[14, -15, -37, 40]$
9	$[0, X, 0]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	$[17, -20, -42, 43]$
10	$[0, X, 0]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	$[18, -19, -41, 44]$
11	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[21, -24, -46, 47]$
12	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[22, -23, -45, 48]$

Table 15: Wyckoff bond: 24d@6c

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	$[-X, -X, Y]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[12, -21]$
13	$[-Y, -X, -X]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	$[25, -43]$
14	$[Y, X, -X]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	$[26, -41]$
15	$[Y, -X, X]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	$[27, -44]$
16	$[-Y, X, X]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	$[28, -42]$
17	$[-X, -Y, -X]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	$[29, -38]$
18	$[-X, Y, X]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	$[30, -40]$
19	$[X, Y, -X]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	$[31, -37]$
20	$[X, -Y, X]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	$[32, -39]$
21	$[-X, -X, -Y]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[33, -48]$
22	$[X, -X, Y]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[34, -46]$
23	$[-X, X, Y]$	$[0, \frac{1}{2}, \frac{1}{4}]$	$[35, -47]$
24	$[X, X, -Y]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[36, -45]$

Table 16: Wyckoff bond: 24e@6c

No.	vector	center	mapping
1	[$X, Y, 0$]	[$\frac{1}{4}, 0, \frac{1}{2}$]	[1,26]
2	[$-X, -Y, 0$]	[$\frac{3}{4}, 0, \frac{1}{2}$]	[2,25]
3	[$-X, Y, 0$]	[$\frac{3}{4}, 0, \frac{1}{2}$]	[3,28]
4	[$X, -Y, 0$]	[$\frac{1}{4}, 0, \frac{1}{2}$]	[4,27]
5	[$0, X, Y$]	[$\frac{1}{2}, \frac{1}{4}, 0$]	[5,30]
6	[$0, -X, -Y$]	[$\frac{1}{2}, \frac{3}{4}, 0$]	[6,29]
7	[$0, -X, Y$]	[$\frac{1}{2}, \frac{3}{4}, 0$]	[7,32]
8	[$0, X, -Y$]	[$\frac{1}{2}, \frac{1}{4}, 0$]	[8,31]
9	[$Y, 0, X$]	[$0, \frac{1}{2}, \frac{1}{4}$]	[9,34]
10	[$-Y, 0, -X$]	[$0, \frac{1}{2}, \frac{3}{4}$]	[10,33]
11	[$Y, 0, -X$]	[$0, \frac{1}{2}, \frac{3}{4}$]	[11,36]
12	[$-Y, 0, X$]	[$0, \frac{1}{2}, \frac{1}{4}$]	[12,35]
13	[$Y, X, 0$]	[$\frac{1}{2}, \frac{3}{4}, 0$]	[13,38]
14	[$-Y, -X, 0$]	[$\frac{1}{2}, \frac{1}{4}, 0$]	[14,37]
15	[$Y, -X, 0$]	[$\frac{1}{2}, \frac{1}{4}, 0$]	[15,40]
16	[$-Y, X, 0$]	[$\frac{1}{2}, \frac{3}{4}, 0$]	[16,39]
17	[$X, 0, -Y$]	[$\frac{3}{4}, 0, \frac{1}{2}$]	[17,42]
18	[$-X, 0, Y$]	[$\frac{1}{4}, 0, \frac{1}{2}$]	[18,41]
19	[$-X, 0, -Y$]	[$\frac{1}{4}, 0, \frac{1}{2}$]	[19,44]
20	[$X, 0, Y$]	[$\frac{3}{4}, 0, \frac{1}{2}$]	[20,43]
21	[$0, Y, -X$]	[$0, \frac{1}{2}, \frac{1}{4}$]	[21,46]
22	[$0, -Y, X$]	[$0, \frac{1}{2}, \frac{3}{4}$]	[22,45]
23	[$0, Y, X$]	[$0, \frac{1}{2}, \frac{1}{4}$]	[23,48]
24	[$0, -Y, -X$]	[$0, \frac{1}{2}, \frac{1}{4}$]	[24,47]

Table 17: Wyckoff bond: 24f@6c

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]
13	[$0, -X, -Y$]	[$\frac{3}{4}, 0, \frac{1}{2}$]	[25,-28]
14	[$0, X, -Y$]	[$\frac{1}{4}, 0, \frac{1}{2}$]	[26,-27]
15	[$-Y, 0, -X$]	[$\frac{1}{2}, \frac{3}{4}, 0$]	[29,-32]

continued ...

Table 17

No.	vector	center	mapping
16	$[-Y, 0, X]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[30, -31]
17	$[-X, -Y, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[33, -36]
18	$[X, -Y, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[34, -35]
19	$[-X, 0, Y]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[37, -40]
20	$[X, 0, Y]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[38, -39]
21	$[0, -Y, X]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[41, -44]
22	$[0, -Y, -X]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[42, -43]
23	$[-Y, -X, 0]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[45, -48]
24	$[-Y, X, 0]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[46, -47]

Table 18: Wyckoff bond: 48g@6c

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]
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]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[27]
28	$[-X, Y, Z]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[29]
30	$[-Z, X, Y]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[30]
31	$[Z, X, -Y]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[31]

continued ...

Table 18

No.	vector	center	mapping
32	$[Z, -X, Y]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[32]
33	$[-Y, -Z, -X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[33]
34	$[Y, -Z, X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[34]
35	$[-Y, Z, X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[35]
36	$[Y, Z, -X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[37]
38	$[Y, X, Z]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2}, \frac{3}{4}, 0]$	[39]
40	$[Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[42]
43	$[X, Z, Y]$	$[\frac{3}{4}, 0, \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{4}, 0, \frac{1}{2}]$	[44]
45	$[-Z, -Y, X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[45]
46	$[-Z, Y, -X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[46]
47	$[Z, -Y, -X]$	$[0, \frac{1}{2}, \frac{1}{4}]$	[47]
48	$[Z, Y, X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	[48]

* Wyckoff site: 6d, site symmetry: $-4\bar{m}.2$

Table 19: Wyckoff bond: 6a@6d

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	[1, 4, -18, -19, 26, 27, -41, -44]
2	$[-X, 0, 0]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	[2, 3, -17, -20, 25, 28, -42, -43]
3	$[0, X, 0]$	$[0, \frac{1}{4}, \frac{1}{2}]$	[5, 8, -14, -15, 30, 31, -37, -40]
4	$[0, -X, 0]$	$[0, \frac{3}{4}, \frac{1}{2}]$	[6, 7, -13, -16, 29, 32, -38, -39]
5	$[0, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[9, 12, -21, -24, 34, 35, -46, -47]
6	$[0, 0, -X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[10, 11, -22, -23, 33, 36, -45, -48]

Table 20: Wyckoff bond: 12b@6d

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]
7	$[0, -X, -X]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	[25, -28, 42, -43]
8	$[0, X, -X]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	[26, -27, -41, 44]
9	$[-X, 0, -X]$	$[0, \frac{3}{4}, \frac{1}{2}]$	[29, -32, -38, 39]

continued ...

Table 20

No.	vector	center	mapping
10	$[-X, 0, X]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[30, -31, 37, -40]$
11	$[-X, -X, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[33, -36, 45, -48]$
12	$[X, -X, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[34, -35, -46, 47]$

Table 21: Wyckoff bond: 12c@6d

No.	vector	center	mapping
1	$[0, 0, X]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[1, -4, -26, 27]$
2	$[0, 0, X]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[2, -3, -25, 28]$
3	$[X, 0, 0]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[5, -8, -30, 31]$
4	$[X, 0, 0]$	$[0, \frac{3}{4}, \frac{1}{2}]$	$[6, -7, -29, 32]$
5	$[0, X, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[9, -12, -34, 35]$
6	$[0, X, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[10, -11, -33, 36]$
7	$[0, 0, -X]$	$[0, \frac{3}{4}, \frac{1}{2}]$	$[13, -16, -38, 39]$
8	$[0, 0, -X]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[14, -15, -37, 40]$
9	$[0, X, 0]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[17, -20, -42, 43]$
10	$[0, X, 0]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[18, -19, -41, 44]$
11	$[X, 0, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[21, -24, -46, 47]$
12	$[X, 0, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[22, -23, -45, 48]$

Table 22: Wyckoff bond: 24d@6d

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	$[-X, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[12, -21]$
13	$[-Y, -X, -X]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[25, -43]$
14	$[Y, X, -X]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[26, -41]$
15	$[Y, -X, X]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[27, -44]$
16	$[-Y, X, X]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[28, -42]$
17	$[-X, -Y, -X]$	$[0, \frac{3}{4}, \frac{1}{2}]$	$[29, -38]$
18	$[-X, Y, X]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[30, -40]$
19	$[X, Y, -X]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[31, -37]$

continued ...

Table 22

No.	vector	center	mapping
20	$[X, -Y, X]$	$[0, \frac{3}{4}, \frac{1}{2}]$	$[32, -39]$
21	$[-X, -X, -Y]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[33, -48]$
22	$[X, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[34, -46]$
23	$[-X, X, Y]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[35, -47]$
24	$[X, X, -Y]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[36, -45]$

Table 23: Wyckoff bond: 24e@6d

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[1, 26]$
2	$[-X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[2, 25]$
3	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[3, 28]$
4	$[X, -Y, 0]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[4, 27]$
5	$[0, X, Y]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[5, 30]$
6	$[0, -X, -Y]$	$[0, \frac{3}{4}, \frac{1}{2}]$	$[6, 29]$
7	$[0, -X, Y]$	$[0, \frac{3}{4}, \frac{1}{2}]$	$[7, 32]$
8	$[0, X, -Y]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[8, 31]$
9	$[Y, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[9, 34]$
10	$[-Y, 0, -X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[10, 33]$
11	$[Y, 0, -X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[11, 36]$
12	$[-Y, 0, X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[12, 35]$
13	$[Y, X, 0]$	$[0, \frac{3}{4}, \frac{1}{2}]$	$[13, 38]$
14	$[-Y, -X, 0]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[14, 37]$
15	$[Y, -X, 0]$	$[0, \frac{1}{4}, \frac{1}{2}]$	$[15, 40]$
16	$[-Y, X, 0]$	$[0, \frac{3}{4}, \frac{1}{2}]$	$[16, 39]$
17	$[X, 0, -Y]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[17, 42]$
18	$[-X, 0, Y]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[18, 41]$
19	$[-X, 0, -Y]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[19, 44]$
20	$[X, 0, Y]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[20, 43]$
21	$[0, Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[21, 46]$
22	$[0, -Y, X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[22, 45]$
23	$[0, Y, X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[23, 48]$
24	$[0, -Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[24, 47]$

Table 24: Wyckoff bond: 24f@6d

No.	vector	center	mapping
1	$[0, X, Y]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[1, -4]$
2	$[0, -X, Y]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[2, -3]$
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	$[X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[9, -12]$

continued ...

Table 24

No.	vector	center	mapping
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]
13	$[0, -X, -Y]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	[25, -28]
14	$[0, X, -Y]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	[26, -27]
15	$[-Y, 0, -X]$	$[0, \frac{3}{4}, \frac{1}{2}]$	[29, -32]
16	$[-Y, 0, X]$	$[0, \frac{1}{4}, \frac{1}{2}]$	[30, -31]
17	$[-X, -Y, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[33, -36]
18	$[X, -Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[34, -35]
19	$[-X, 0, Y]$	$[0, \frac{1}{4}, \frac{1}{2}]$	[37, -40]
20	$[X, 0, Y]$	$[0, \frac{3}{4}, \frac{1}{2}]$	[38, -39]
21	$[0, -Y, X]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	[41, -44]
22	$[0, -Y, -X]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	[42, -43]
23	$[-Y, -X, 0]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[45, -48]
24	$[-Y, X, 0]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[46, -47]

Table 25: Wyckoff bond: 48g@6d

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]

continued ...

Table 25

No.	vector	center	mapping
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]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	[27]
28	$[-X, Y, Z]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	[28]
29	$[-Z, -X, -Y]$	$[0, \frac{3}{4}, \frac{1}{2}]$	[29]
30	$[-Z, X, Y]$	$[0, \frac{1}{4}, \frac{1}{2}]$	[30]
31	$[Z, X, -Y]$	$[0, \frac{1}{4}, \frac{1}{2}]$	[31]
32	$[Z, -X, Y]$	$[0, \frac{3}{4}, \frac{1}{2}]$	[32]
33	$[-Y, -Z, -X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[33]
34	$[Y, -Z, X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[34]
35	$[-Y, Z, X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[35]
36	$[Y, Z, -X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[36]
37	$[-Y, -X, Z]$	$[0, \frac{1}{4}, \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[0, \frac{3}{4}, \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[0, \frac{3}{4}, \frac{1}{2}]$	[39]
40	$[Y, -X, -Z]$	$[0, \frac{1}{4}, \frac{1}{2}]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	[41]
42	$[X, -Z, -Y]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	[42]
43	$[X, Z, Y]$	$[\frac{3}{4}, \frac{1}{2}, 0]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{4}, \frac{1}{2}, 0]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[46]
47	$[Z, -Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{4}]$	[47]
48	$[Z, Y, X]$	$[\frac{1}{2}, 0, \frac{3}{4}]$	[48]

* Wyckoff site: **8e**, site symmetry: .32

Table 26: Wyckoff bond: 8a@8e

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]
5	$[-X, -X, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25,29,33,-38,-43,-48]
6	$[X, X, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[26,31,36,-37,-41,-45]
7	$[X, -X, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[27,32,34,-39,-44,-46]
8	$[-X, X, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[28,30,35,-40,-42,-47]

Table 27: Wyckoff bond: 24b@8e

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]
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]
13	[-X, -X, -Y]	[$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$]	[25, -38]
14	[X, X, -Y]	[$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$]	[26, -37]
15	[X, -X, Y]	[$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$]	[27, -39]
16	[-X, X, Y]	[$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$]	[28, -40]
17	[-Y, -X, -X]	[$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$]	[29, -48]
18	[-Y, X, X]	[$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$]	[30, -47]
19	[Y, X, -X]	[$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$]	[31, -45]
20	[Y, -X, X]	[$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$]	[32, -46]
21	[-X, -Y, -X]	[$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$]	[33, -43]
22	[X, -Y, X]	[$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$]	[34, -44]
23	[-X, Y, X]	[$\frac{3}{4}, \frac{1}{4}, \frac{1}{4}$]	[35, -42]
24	[X, Y, -X]	[$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$]	[36, -41]

Table 28: Wyckoff bond: 24c@8e

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]
13	[-X, X, 0]	[$\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$]	[25, 38]
14	[X, -X, 0]	[$\frac{1}{4}, \frac{1}{4}, \frac{3}{4}$]	[26, 37]
15	[X, X, 0]	[$\frac{1}{4}, \frac{3}{4}, \frac{1}{4}$]	[27, 39]

continued ...

Table 28

No.	vector	center	mapping
16	$[-X, -X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[28,40]
17	$[0, -X, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[29,48]
18	$[0, X, -X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[30,47]
19	$[0, X, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[31,45]
20	$[0, -X, -X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[32,46]
21	$[X, 0, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[33,43]
22	$[-X, 0, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[34,44]
23	$[X, 0, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[35,42]
24	$[-X, 0, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[36,41]

Table 29: Wyckoff bond: 48d@8e

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	$[Y, X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[14]
15	$[Y, -X, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[15]
16	$[-Y, X, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[16]
17	$[X, Z, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[19]
20	$[X, -Z, Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[20]
21	$[Z, Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[21]
22	$[Z, -Y, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[27]
28	$[-X, Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[29]
30	$[-Z, X, Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[30]
31	$[Z, X, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[31]

continued ...

Table 29

No.	vector	center	mapping
32	$[Z, -X, Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[32]
33	$[-Y, -Z, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[33]
34	$[Y, -Z, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[34]
35	$[-Y, Z, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[35]
36	$[Y, Z, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[37]
38	$[Y, X, Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[39]
40	$[Y, -X, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[42]
43	$[X, Z, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[46]
47	$[Z, -Y, -X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[47]
48	$[Z, Y, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[48]

* Wyckoff site: 12f, site symmetry: mm2..

Table 30: Wyckoff bond: 12a@12f

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	[1,4,26,27]
2	$[-X, 0, 0]$	$[-x, 0, 0]$	[2,3,25,28]
3	$[0, X, 0]$	$[0, x, 0]$	[5,8,30,31]
4	$[0, -X, 0]$	$[0, -x, 0]$	[6,7,29,32]
5	$[0, 0, X]$	$[0, 0, x]$	[9,12,34,35]
6	$[0, 0, -X]$	$[0, 0, -x]$	[10,11,33,36]
7	$[0, X, 0]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[13,16,38,39]
8	$[0, -X, 0]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[14,15,37,40]
9	$[X, 0, 0]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[17,20,42,43]
10	$[-X, 0, 0]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[18,19,41,44]
11	$[0, 0, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[21,24,46,47]
12	$[0, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[22,23,45,48]

Table 31: Wyckoff bond: 12b@12f

No.	vector	center	mapping
1	$[0, 0, X]$	$[x, 0, 0]$	[1,-4,-26,27]
2	$[0, 0, X]$	$[-x, 0, 0]$	[2,-3,-25,28]
3	$[X, 0, 0]$	$[0, x, 0]$	[5,-8,-30,31]

continued ...

Table 31

No.	vector	center	mapping
4	$[X, 0, 0]$	$[0, -x, 0]$	$[6, -7, -29, 32]$
5	$[0, X, 0]$	$[0, 0, x]$	$[9, -12, -34, 35]$
6	$[0, X, 0]$	$[0, 0, -x]$	$[10, -11, -33, 36]$
7	$[0, 0, -X]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[13, -16, -38, 39]$
8	$[0, 0, -X]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	$[14, -15, -37, 40]$
9	$[0, X, 0]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[17, -20, -42, 43]$
10	$[0, X, 0]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	$[18, -19, -41, 44]$
11	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	$[21, -24, -46, 47]$
12	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	$[22, -23, -45, 48]$

Table 32: Wyckoff bond: 12c@12f

No.	vector	center	mapping
1	$[0, X, 0]$	$[x, 0, 0]$	$[1, -4, 26, -27]$
2	$[0, -X, 0]$	$[-x, 0, 0]$	$[2, -3, 25, -28]$
3	$[0, 0, X]$	$[0, x, 0]$	$[5, -8, 30, -31]$
4	$[0, 0, -X]$	$[0, -x, 0]$	$[6, -7, 29, -32]$
5	$[X, 0, 0]$	$[0, 0, x]$	$[9, -12, 34, -35]$
6	$[-X, 0, 0]$	$[0, 0, -x]$	$[10, -11, 33, -36]$
7	$[X, 0, 0]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[13, -16, 38, -39]$
8	$[-X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	$[14, -15, 37, -40]$
9	$[0, 0, -X]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[17, -20, 42, -43]$
10	$[0, 0, X]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	$[18, -19, 41, -44]$
11	$[0, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	$[21, -24, 46, -47]$
12	$[0, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	$[22, -23, 45, -48]$

Table 33: Wyckoff bond: 24d@12f

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, 0, 0]$	$[1, 26]$
2	$[-X, -Y, 0]$	$[-x, 0, 0]$	$[2, 25]$
3	$[-X, Y, 0]$	$[-x, 0, 0]$	$[3, 28]$
4	$[X, -Y, 0]$	$[x, 0, 0]$	$[4, 27]$
5	$[0, X, Y]$	$[0, x, 0]$	$[5, 30]$
6	$[0, -X, -Y]$	$[0, -x, 0]$	$[6, 29]$
7	$[0, -X, Y]$	$[0, -x, 0]$	$[7, 32]$
8	$[0, X, -Y]$	$[0, x, 0]$	$[8, 31]$
9	$[Y, 0, X]$	$[0, 0, x]$	$[9, 34]$
10	$[-Y, 0, -X]$	$[0, 0, -x]$	$[10, 33]$
11	$[Y, 0, -X]$	$[0, 0, -x]$	$[11, 36]$
12	$[-Y, 0, X]$	$[0, 0, x]$	$[12, 35]$
13	$[Y, X, 0]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[13, 38]$

continued ...

Table 33

No.	vector	center	mapping
14	$[-Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[14,37]
15	$[Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[15,40]
16	$[-Y, X, 0]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[16,39]
17	$[X, 0, -Y]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[17,42]
18	$[-X, 0, Y]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[18,41]
19	$[-X, 0, -Y]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[19,44]
20	$[X, 0, Y]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[20,43]
21	$[0, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[21,46]
22	$[0, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[22,45]
23	$[0, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[23,48]
24	$[0, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[24,47]

Table 34: Wyckoff bond: 24e@12f

No.	vector	center	mapping
1	$[Y, 0, X]$	$[x, 0, 0]$	[1,27]
2	$[-Y, 0, X]$	$[-x, 0, 0]$	[2,28]
3	$[-Y, 0, -X]$	$[-x, 0, 0]$	[3,25]
4	$[Y, 0, -X]$	$[x, 0, 0]$	[4,26]
5	$[X, Y, 0]$	$[0, x, 0]$	[5,31]
6	$[X, -Y, 0]$	$[0, -x, 0]$	[6,32]
7	$[-X, -Y, 0]$	$[0, -x, 0]$	[7,29]
8	$[-X, Y, 0]$	$[0, x, 0]$	[8,30]
9	$[0, X, Y]$	$[0, 0, x]$	[9,35]
10	$[0, X, -Y]$	$[0, 0, -x]$	[10,36]
11	$[0, -X, -Y]$	$[0, 0, -x]$	[11,33]
12	$[0, -X, Y]$	$[0, 0, x]$	[12,34]
13	$[0, Y, -X]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[13,39]
14	$[0, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[14,40]
15	$[0, -Y, X]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[15,37]
16	$[0, Y, X]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[16,38]
17	$[Y, X, 0]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[17,43]
18	$[-Y, X, 0]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[18,44]
19	$[-Y, -X, 0]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[19,41]
20	$[Y, -X, 0]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[20,42]
21	$[X, 0, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[21,47]
22	$[X, 0, Y]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[22,48]
23	$[-X, 0, Y]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[23,45]
24	$[-X, 0, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[24,46]

Table 35: Wyckoff bond: 24f@12f

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]
13	[0, -X, -Y]	[-x, 0, 0]	[25, -28]
14	[0, X, -Y]	[x, 0, 0]	[26, -27]
15	[-Y, 0, -X]	[0, -x, 0]	[29, -32]
16	[-Y, 0, X]	[0, x, 0]	[30, -31]
17	[-X, -Y, 0]	[0, 0, -x]	[33, -36]
18	[X, -Y, 0]	[0, 0, x]	[34, -35]
19	[-X, 0, Y]	[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]	[37, -40]
20	[X, 0, Y]	[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]	[38, -39]
21	[0, -Y, X]	[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]	[41, -44]
22	[0, -Y, -X]	[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[42, -43]
23	[-Y, -X, 0]	[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]	[45, -48]
24	[-Y, X, 0]	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]	[46, -47]

Table 36: Wyckoff bond: 48g@12f

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]	[\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]

continued ...

Table 36

No.	vector	center	mapping
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]
25	$[-X, -Y, -Z]$	$[-x, 0, 0]$	[25]
26	$[X, Y, -Z]$	$[x, 0, 0]$	[26]
27	$[X, -Y, Z]$	$[x, 0, 0]$	[27]
28	$[-X, Y, Z]$	$[-x, 0, 0]$	[28]
29	$[-Z, -X, -Y]$	$[0, -x, 0]$	[29]
30	$[-Z, X, Y]$	$[0, x, 0]$	[30]
31	$[Z, X, -Y]$	$[0, x, 0]$	[31]
32	$[Z, -X, Y]$	$[0, -x, 0]$	[32]
33	$[-Y, -Z, -X]$	$[0, 0, -x]$	[33]
34	$[Y, -Z, X]$	$[0, 0, x]$	[34]
35	$[-Y, Z, X]$	$[0, 0, x]$	[35]
36	$[Y, Z, -X]$	$[0, 0, -x]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[39]
40	$[Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[46]
47	$[Z, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[47]
48	$[Z, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[48]

* Wyckoff site: 12g, site symmetry: mm2..

Table 37: Wyckoff bond: 12a@12g

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, \frac{1}{2}]$	[1,4,26,27]
2	$[-X, 0, 0]$	$[-x, 0, \frac{1}{2}]$	[2,3,25,28]
3	$[0, X, 0]$	$[\frac{1}{2}, x, 0]$	[5,8,30,31]
4	$[0, -X, 0]$	$[\frac{1}{2}, -x, 0]$	[6,7,29,32]
5	$[0, 0, X]$	$[0, \frac{1}{2}, x]$	[9,12,34,35]
6	$[0, 0, -X]$	$[0, \frac{1}{2}, -x]$	[10,11,33,36]

continued ...

Table 37

No.	vector	center	mapping
7	$[0, X, 0]$	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	$[13, 16, 38, 39]$
8	$[0, -X, 0]$	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	$[14, 15, 37, 40]$
9	$[X, 0, 0]$	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	$[17, 20, 42, 43]$
10	$[-X, 0, 0]$	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	$[18, 19, 41, 44]$
11	$[0, 0, -X]$	$[0, \frac{1}{2}, \frac{1}{2} - x]$	$[21, 24, 46, 47]$
12	$[0, 0, X]$	$[0, \frac{1}{2}, x + \frac{1}{2}]$	$[22, 23, 45, 48]$

Table 38: Wyckoff bond: 12b@12g

No.	vector	center	mapping
1	$[0, 0, X]$	$[x, 0, \frac{1}{2}]$	$[1, -4, -26, 27]$
2	$[0, 0, X]$	$[-x, 0, \frac{1}{2}]$	$[2, -3, -25, 28]$
3	$[X, 0, 0]$	$[\frac{1}{2}, x, 0]$	$[5, -8, -30, 31]$
4	$[X, 0, 0]$	$[\frac{1}{2}, -x, 0]$	$[6, -7, -29, 32]$
5	$[0, X, 0]$	$[0, \frac{1}{2}, x]$	$[9, -12, -34, 35]$
6	$[0, X, 0]$	$[0, \frac{1}{2}, -x]$	$[10, -11, -33, 36]$
7	$[0, 0, -X]$	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	$[13, -16, -38, 39]$
8	$[0, 0, -X]$	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	$[14, -15, -37, 40]$
9	$[0, X, 0]$	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	$[17, -20, -42, 43]$
10	$[0, X, 0]$	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	$[18, -19, -41, 44]$
11	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{1}{2} - x]$	$[21, -24, -46, 47]$
12	$[X, 0, 0]$	$[0, \frac{1}{2}, x + \frac{1}{2}]$	$[22, -23, -45, 48]$

Table 39: Wyckoff bond: 24c@12g

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, 0, \frac{1}{2}]$	$[1, 26]$
2	$[-X, -Y, 0]$	$[-x, 0, \frac{1}{2}]$	$[2, 25]$
3	$[-X, Y, 0]$	$[-x, 0, \frac{1}{2}]$	$[3, 28]$
4	$[X, -Y, 0]$	$[x, 0, \frac{1}{2}]$	$[4, 27]$
5	$[0, X, Y]$	$[\frac{1}{2}, x, 0]$	$[5, 30]$
6	$[0, -X, -Y]$	$[\frac{1}{2}, -x, 0]$	$[6, 29]$
7	$[0, -X, Y]$	$[\frac{1}{2}, -x, 0]$	$[7, 32]$
8	$[0, X, -Y]$	$[\frac{1}{2}, x, 0]$	$[8, 31]$
9	$[Y, 0, X]$	$[0, \frac{1}{2}, x]$	$[9, 34]$
10	$[-Y, 0, -X]$	$[0, \frac{1}{2}, -x]$	$[10, 33]$
11	$[Y, 0, -X]$	$[0, \frac{1}{2}, -x]$	$[11, 36]$
12	$[-Y, 0, X]$	$[0, \frac{1}{2}, x]$	$[12, 35]$
13	$[Y, X, 0]$	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	$[13, 38]$
14	$[-Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	$[14, 37]$
15	$[Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	$[15, 40]$
16	$[-Y, X, 0]$	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	$[16, 39]$

continued ...

Table 39

No.	vector	center	mapping
17	$[X, 0, -Y]$	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[17, 42]
18	$[-X, 0, Y]$	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[18, 41]
19	$[-X, 0, -Y]$	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[19, 44]
20	$[X, 0, Y]$	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[20, 43]
21	$[0, Y, -X]$	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[21, 46]
22	$[0, -Y, X]$	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[22, 45]
23	$[0, Y, X]$	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[23, 48]
24	$[0, -Y, -X]$	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[24, 47]

Table 40: Wyckoff bond: 24d@12g

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]
13	$[0, -X, -Y]$	$[-x, 0, \frac{1}{2}]$	[25, -28]
14	$[0, X, -Y]$	$[x, 0, \frac{1}{2}]$	[26, -27]
15	$[-Y, 0, -X]$	$[\frac{1}{2}, -x, 0]$	[29, -32]
16	$[-Y, 0, X]$	$[\frac{1}{2}, x, 0]$	[30, -31]
17	$[-X, -Y, 0]$	$[0, \frac{1}{2}, -x]$	[33, -36]
18	$[X, -Y, 0]$	$[0, \frac{1}{2}, x]$	[34, -35]
19	$[-X, 0, Y]$	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[37, -40]
20	$[X, 0, Y]$	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[38, -39]
21	$[0, -Y, X]$	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[41, -44]
22	$[0, -Y, -X]$	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[42, -43]
23	$[-Y, -X, 0]$	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[45, -48]
24	$[-Y, X, 0]$	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[46, -47]

Table 41: Wyckoff bond: 48e@12g

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

continued ...

Table 41

No.	vector	center	mapping
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]
25	$[-X, -Y, -Z]$	$[-x, 0, \frac{1}{2}]$	[25]
26	$[X, Y, -Z]$	$[x, 0, \frac{1}{2}]$	[26]
27	$[X, -Y, Z]$	$[x, 0, \frac{1}{2}]$	[27]
28	$[-X, Y, Z]$	$[-x, 0, \frac{1}{2}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{1}{2}, -x, 0]$	[29]
30	$[-Z, X, Y]$	$[\frac{1}{2}, x, 0]$	[30]
31	$[Z, X, -Y]$	$[\frac{1}{2}, x, 0]$	[31]
32	$[Z, -X, Y]$	$[\frac{1}{2}, -x, 0]$	[32]
33	$[-Y, -Z, -X]$	$[0, \frac{1}{2}, -x]$	[33]
34	$[Y, -Z, X]$	$[0, \frac{1}{2}, x]$	[34]
35	$[-Y, Z, X]$	$[0, \frac{1}{2}, x]$	[35]
36	$[Y, Z, -X]$	$[0, \frac{1}{2}, -x]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[37]
38	$[Y, X, Z]$	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[39]
40	$[Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[44]
45	$[-Z, -Y, X]$	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[46]
47	$[Z, -Y, -X]$	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[47]
48	$[Z, Y, X]$	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[48]

* Wyckoff site: 12h, site symmetry: mm2..

Table 42: Wyckoff bond: 12a@12h

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, \frac{1}{2}, 0]$	[1,4,26,27]
2	$[-X, 0, 0]$	$[-x, \frac{1}{2}, 0]$	[2,3,25,28]
3	$[0, X, 0]$	$[0, x, \frac{1}{2}]$	[5,8,30,31]
4	$[0, -X, 0]$	$[0, -x, \frac{1}{2}]$	[6,7,29,32]
5	$[0, 0, X]$	$[\frac{1}{2}, 0, x]$	[9,12,34,35]
6	$[0, 0, -X]$	$[\frac{1}{2}, 0, -x]$	[10,11,33,36]
7	$[0, X, 0]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[13,16,38,39]
8	$[0, -X, 0]$	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[14,15,37,40]
9	$[X, 0, 0]$	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[17,20,42,43]
10	$[-X, 0, 0]$	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[18,19,41,44]
11	$[0, 0, -X]$	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[21,24,46,47]
12	$[0, 0, X]$	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[22,23,45,48]

Table 43: Wyckoff bond: 12b@12h

No.	vector	center	mapping
1	$[0, 0, X]$	$[x, \frac{1}{2}, 0]$	[1,-4,-26,27]
2	$[0, 0, X]$	$[-x, \frac{1}{2}, 0]$	[2,-3,-25,28]
3	$[X, 0, 0]$	$[0, x, \frac{1}{2}]$	[5,-8,-30,31]
4	$[X, 0, 0]$	$[0, -x, \frac{1}{2}]$	[6,-7,-29,32]
5	$[0, X, 0]$	$[\frac{1}{2}, 0, x]$	[9,-12,-34,35]
6	$[0, X, 0]$	$[\frac{1}{2}, 0, -x]$	[10,-11,-33,36]
7	$[0, 0, -X]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[13,-16,-38,39]
8	$[0, 0, -X]$	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[14,-15,-37,40]
9	$[0, X, 0]$	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[17,-20,-42,43]
10	$[0, X, 0]$	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[18,-19,-41,44]
11	$[X, 0, 0]$	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[21,-24,-46,47]
12	$[X, 0, 0]$	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[22,-23,-45,48]

Table 44: Wyckoff bond: 24c@12h

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, \frac{1}{2}, 0]$	[1,26]
2	$[-X, -Y, 0]$	$[-x, \frac{1}{2}, 0]$	[2,25]
3	$[-X, Y, 0]$	$[-x, \frac{1}{2}, 0]$	[3,28]
4	$[X, -Y, 0]$	$[x, \frac{1}{2}, 0]$	[4,27]
5	$[0, X, Y]$	$[0, x, \frac{1}{2}]$	[5,30]
6	$[0, -X, -Y]$	$[0, -x, \frac{1}{2}]$	[6,29]

continued ...

Table 44

No.	vector	center	mapping
7	$[0, -X, Y]$	$[0, -x, \frac{1}{2}]$	[7,32]
8	$[0, X, -Y]$	$[0, x, \frac{1}{2}]$	[8,31]
9	$[Y, 0, X]$	$[\frac{1}{2}, 0, x]$	[9,34]
10	$[-Y, 0, -X]$	$[\frac{1}{2}, 0, -x]$	[10,33]
11	$[Y, 0, -X]$	$[\frac{1}{2}, 0, -x]$	[11,36]
12	$[-Y, 0, X]$	$[\frac{1}{2}, 0, x]$	[12,35]
13	$[Y, X, 0]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[13,38]
14	$[-Y, -X, 0]$	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[14,37]
15	$[Y, -X, 0]$	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[15,40]
16	$[-Y, X, 0]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[16,39]
17	$[X, 0, -Y]$	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[17,42]
18	$[-X, 0, Y]$	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[18,41]
19	$[-X, 0, -Y]$	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[19,44]
20	$[X, 0, Y]$	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[20,43]
21	$[0, Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[21,46]
22	$[0, -Y, X]$	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[22,45]
23	$[0, Y, X]$	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[23,48]
24	$[0, -Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[24,47]

Table 45: Wyckoff bond: 24d@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	$[X, 0, -Y]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[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]
13	$[0, -X, -Y]$	$[-x, \frac{1}{2}, 0]$	[25,-28]
14	$[0, X, -Y]$	$[x, \frac{1}{2}, 0]$	[26,-27]
15	$[-Y, 0, -X]$	$[0, -x, \frac{1}{2}]$	[29,-32]
16	$[-Y, 0, X]$	$[0, x, \frac{1}{2}]$	[30,-31]
17	$[-X, -Y, 0]$	$[\frac{1}{2}, 0, -x]$	[33,-36]
18	$[X, -Y, 0]$	$[\frac{1}{2}, 0, x]$	[34,-35]
19	$[-X, 0, Y]$	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[37,-40]
20	$[X, 0, Y]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[38,-39]
21	$[0, -Y, X]$	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[41,-44]
22	$[0, -Y, -X]$	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[42,-43]

continued ...

Table 45

No.	vector	center	mapping
23	$[-Y, -X, 0]$	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[45, -48]
24	$[-Y, X, 0]$	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[46, -47]

Table 46: Wyckoff bond: 48e@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]
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	$[Y, X, -Z]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[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]
25	$[-X, -Y, -Z]$	$[-x, \frac{1}{2}, 0]$	[25]
26	$[X, Y, -Z]$	$[x, \frac{1}{2}, 0]$	[26]
27	$[X, -Y, Z]$	$[x, \frac{1}{2}, 0]$	[27]
28	$[-X, Y, Z]$	$[-x, \frac{1}{2}, 0]$	[28]
29	$[-Z, -X, -Y]$	$[0, -x, \frac{1}{2}]$	[29]
30	$[-Z, X, Y]$	$[0, x, \frac{1}{2}]$	[30]
31	$[Z, X, -Y]$	$[0, x, \frac{1}{2}]$	[31]
32	$[Z, -X, Y]$	$[0, -x, \frac{1}{2}]$	[32]
33	$[-Y, -Z, -X]$	$[\frac{1}{2}, 0, -x]$	[33]
34	$[Y, -Z, X]$	$[\frac{1}{2}, 0, x]$	[34]
35	$[-Y, Z, X]$	$[\frac{1}{2}, 0, x]$	[35]
36	$[Y, Z, -X]$	$[\frac{1}{2}, 0, -x]$	[36]
37	$[-Y, -X, Z]$	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[38]

continued ...

Table 46

No.	vector	center	mapping
39	$[-Y, X, -Z]$	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[39]
40	$[Y, -X, -Z]$	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[46]
47	$[Z, -Y, -X]$	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[47]
48	$[Z, Y, X]$	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[48]

* Wyckoff site: 16i, site symmetry: .3.

Table 47: Wyckoff bond: 16a@16i

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	$[X, X, -X]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[13,17,21]
6	$[-X, -X, -X]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[14,19,24]
7	$[X, -X, X]$	$[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[15,20,22]
8	$[-X, X, X]$	$[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}]$	[16,18,23]
9	$[-X, -X, -X]$	$[-x, -x, -x]$	[25,29,33]
10	$[X, X, -X]$	$[x, x, -x]$	[26,31,36]
11	$[X, -X, X]$	$[x, -x, x]$	[27,32,34]
12	$[-X, X, X]$	$[-x, x, x]$	[28,30,35]
13	$[-X, -X, X]$	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[37,41,45]
14	$[X, X, X]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[38,43,48]
15	$[-X, X, -X]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[39,44,46]
16	$[X, -X, -X]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[40,42,47]

Table 48: Wyckoff bond: 48b@16i

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]

continued ...

Table 48

No.	vector	center	mapping
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	$[Y, X, -Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[14]
15	$[Y, -X, Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[15]
16	$[-Y, X, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}]$	[16]
17	$[X, Z, -Y]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[19]
20	$[X, -Z, Y]$	$[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[20]
21	$[Z, Y, -X]$	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[21]
22	$[Z, -Y, X]$	$[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, -x, -x]$	[25]
26	$[X, Y, -Z]$	$[x, x, -x]$	[26]
27	$[X, -Y, Z]$	$[x, -x, x]$	[27]
28	$[-X, Y, Z]$	$[-x, x, x]$	[28]
29	$[-Z, -X, -Y]$	$[-x, -x, -x]$	[29]
30	$[-Z, X, Y]$	$[-x, x, x]$	[30]
31	$[Z, X, -Y]$	$[x, x, -x]$	[31]
32	$[Z, -X, Y]$	$[x, -x, x]$	[32]
33	$[-Y, -Z, -X]$	$[-x, -x, -x]$	[33]
34	$[Y, -Z, X]$	$[x, -x, x]$	[34]
35	$[-Y, Z, X]$	$[-x, x, x]$	[35]
36	$[Y, Z, -X]$	$[x, x, -x]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[39]
40	$[Y, -X, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[46]
47	$[Z, -Y, -X]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[47]
48	$[Z, Y, X]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[48]

* Wyckoff site: 24j, site symmetry: ..2

Table 49: Wyckoff bond: 24a@24j

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	$[-Y, X, X]$	$[\frac{3}{4}, y, \frac{1}{2} - y]$	$[3, -17]$
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	$[-X, X, Y]$	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	$[12, -24]$
13	$[-Y, -X, X]$	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	$[25, -42]$
14	$[Y, X, X]$	$[\frac{1}{4}, y, \frac{1}{2} - y]$	$[26, -44]$
15	$[Y, -X, -X]$	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	$[27, -41]$
16	$[-Y, X, -X]$	$[\frac{3}{4}, y, y + \frac{1}{2}]$	$[28, -43]$
17	$[X, -Y, -X]$	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	$[29, -39]$
18	$[X, Y, X]$	$[\frac{1}{2} - y, \frac{1}{4}, y]$	$[30, -37]$
19	$[-X, Y, -X]$	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	$[31, -40]$
20	$[-X, -Y, X]$	$[y + \frac{1}{2}, \frac{3}{4}, y]$	$[32, -38]$
21	$[-X, X, -Y]$	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	$[33, -45]$
22	$[X, X, Y]$	$[y, \frac{1}{2} - y, \frac{1}{4}]$	$[34, -47]$
23	$[-X, -X, Y]$	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	$[35, -46]$
24	$[X, -X, -Y]$	$[y, y + \frac{1}{2}, \frac{3}{4}]$	$[36, -48]$

Table 50: Wyckoff bond: 24b@24j

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	$[-X, -X, 0]$	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	$[12, 24]$
13	$[0, -X, -X]$	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	$[25, 42]$
14	$[0, X, -X]$	$[\frac{1}{4}, y, \frac{1}{2} - y]$	$[26, 44]$
15	$[0, -X, X]$	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	$[27, 41]$

continued ...

Table 50

No.	vector	center	mapping
16	$[0, X, X]$	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[28,43]
17	$[-X, 0, -X]$	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[29,39]
18	$[-X, 0, X]$	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[30,37]
19	$[X, 0, -X]$	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[31,40]
20	$[X, 0, X]$	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[32,38]
21	$[-X, -X, 0]$	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[33,45]
22	$[X, -X, 0]$	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[34,47]
23	$[-X, X, 0]$	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[35,46]
24	$[X, X, 0]$	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[36,48]

Table 51: Wyckoff bond: 48c@24j

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]
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]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[27]
28	$[-X, Y, Z]$	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[29]
30	$[-Z, X, Y]$	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[30]
31	$[Z, X, -Y]$	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[31]

continued ...

Table 51

No.	vector	center	mapping
32	$[Z, -X, Y]$	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[33]
34	$[Y, -Z, X]$	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[34]
35	$[-Y, Z, X]$	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[35]
36	$[Y, Z, -X]$	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[37]
38	$[Y, X, Z]$	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[39]
40	$[Y, -X, -Z]$	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[42]
43	$[X, Z, Y]$	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[44]
45	$[-Z, -Y, X]$	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[45]
46	$[-Z, Y, -X]$	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[46]
47	$[Z, -Y, -X]$	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[47]
48	$[Z, Y, X]$	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[48]

* Wyckoff site: 24k, site symmetry: m..

Table 52: Wyckoff bond: 24a@24k

No.	vector	center	mapping
1	$[0, X, Y]$	$[0, y, z]$	[1,28]
2	$[0, -X, Y]$	$[0, -y, z]$	[2,27]
3	$[0, X, -Y]$	$[0, y, -z]$	[3,26]
4	$[0, -X, -Y]$	$[0, -y, -z]$	[4,25]
5	$[Y, 0, X]$	$[z, 0, y]$	[5,32]
6	$[Y, 0, -X]$	$[z, 0, -y]$	[6,31]
7	$[-Y, 0, X]$	$[-z, 0, y]$	[7,30]
8	$[-Y, 0, -X]$	$[-z, 0, -y]$	[8,29]
9	$[X, Y, 0]$	$[y, z, 0]$	[9,36]
10	$[-X, Y, 0]$	$[-y, z, 0]$	[10,35]
11	$[X, -Y, 0]$	$[y, -z, 0]$	[11,34]
12	$[-X, -Y, 0]$	$[-y, -z, 0]$	[12,33]
13	$[X, 0, -Y]$	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[13,40]
14	$[-X, 0, -Y]$	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - z]$	[14,39]
15	$[X, 0, Y]$	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[15,38]
16	$[-X, 0, Y]$	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	[16,37]
17	$[0, Y, -X]$	$[\frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[17,44]
18	$[0, Y, X]$	$[\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[18,43]
19	$[0, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[19,42]
20	$[0, -Y, X]$	$[\frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[20,41]
21	$[Y, X, 0]$	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[21,48]
22	$[Y, -X, 0]$	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[22,47]

continued ...

Table 52

No.	vector	center	mapping
23	$[-Y, X, 0]$	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2}]$	[23,46]
24	$[-Y, -X, 0]$	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2}]$	[24,45]

Table 53: Wyckoff bond: 24b@24k

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	[1,-28]
2	$[-X, 0, 0]$	$[0, -y, z]$	[2,-27]
3	$[-X, 0, 0]$	$[0, y, -z]$	[3,-26]
4	$[X, 0, 0]$	$[0, -y, -z]$	[4,-25]
5	$[0, X, 0]$	$[z, 0, y]$	[5,-32]
6	$[0, -X, 0]$	$[z, 0, -y]$	[6,-31]
7	$[0, -X, 0]$	$[-z, 0, y]$	[7,-30]
8	$[0, X, 0]$	$[-z, 0, -y]$	[8,-29]
9	$[0, 0, X]$	$[y, z, 0]$	[9,-36]
10	$[0, 0, -X]$	$[-y, z, 0]$	[10,-35]
11	$[0, 0, -X]$	$[y, -z, 0]$	[11,-34]
12	$[0, 0, X]$	$[-y, -z, 0]$	[12,-33]
13	$[0, X, 0]$	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[13,-40]
14	$[0, -X, 0]$	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - z]$	[14,-39]
15	$[0, -X, 0]$	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[15,-38]
16	$[0, X, 0]$	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	[16,-37]
17	$[X, 0, 0]$	$[\frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[17,-44]
18	$[-X, 0, 0]$	$[\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[18,-43]
19	$[-X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[19,-42]
20	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[20,-41]
21	$[0, 0, -X]$	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[21,-48]
22	$[0, 0, X]$	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[22,-47]
23	$[0, 0, X]$	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2}]$	[23,-46]
24	$[0, 0, -X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2}]$	[24,-45]

Table 54: Wyckoff bond: 48c@24k

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, z]$	[1]
2	$[-X, -Y, Z]$	$[0, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[0, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[0, -y, -z]$	[4]
5	$[Z, X, Y]$	$[z, 0, y]$	[5]
6	$[Z, -X, -Y]$	$[z, 0, -y]$	[6]
7	$[-Z, -X, Y]$	$[-z, 0, y]$	[7]
8	$[-Z, X, -Y]$	$[-z, 0, -y]$	[8]

continued ...

Table 54

No.	vector	center	mapping
9	[Y, Z, X]	[y, z, 0]	[9]
10	[-Y, Z, -X]	[-y, z, 0]	[10]
11	[Y, -Z, -X]	[y, -z, 0]	[11]
12	[-Y, -Z, X]	[-y, -z, 0]	[12]
13	[Y, X, -Z]	[y + 1/2, 1/2, 1/2 - z]	[13]
14	[-Y, -X, -Z]	[-y + 1/2, 1/2, 1/2 - z]	[14]
15	[Y, -X, Z]	[y + 1/2, 1/2, z + 1/2]	[15]
16	[-Y, X, Z]	[-y + 1/2, 1/2, z + 1/2]	[16]
17	[X, Z, -Y]	[1/2, z + 1/2, 1/2 - y]	[17]
18	[-X, Z, Y]	[-1/2, z + 1/2, y + 1/2]	[18]
19	[-X, -Z, -Y]	[-1/2, 1/2 - z, 1/2 - y]	[19]
20	[X, -Z, Y]	[1/2, 1/2 - z, y + 1/2]	[20]
21	[Z, Y, -X]	[z + 1/2, y + 1/2, 1/2]	[21]
22	[Z, -Y, X]	[z + 1/2, 1/2 - y, 1/2]	[22]
23	[-Z, Y, X]	[-1/2 - z, y + 1/2, 1/2]	[23]
24	[-Z, -Y, -X]	[-1/2 - z, 1/2 - y, 1/2]	[24]
25	[-X, -Y, -Z]	[0, -y, -z]	[25]
26	[X, Y, -Z]	[0, y, -z]	[26]
27	[X, -Y, Z]	[0, -y, z]	[27]
28	[-X, Y, Z]	[0, y, z]	[28]
29	[-Z, -X, -Y]	[-z, 0, -y]	[29]
30	[-Z, X, Y]	[-z, 0, y]	[30]
31	[Z, X, -Y]	[z, 0, -y]	[31]
32	[Z, -X, Y]	[z, 0, y]	[32]
33	[-Y, -Z, -X]	[-y, -z, 0]	[33]
34	[Y, -Z, X]	[y, -z, 0]	[34]
35	[-Y, Z, X]	[-y, z, 0]	[35]
36	[Y, Z, -X]	[y, z, 0]	[36]
37	[-Y, -X, Z]	[-y + 1/2, 1/2, z + 1/2]	[37]
38	[Y, X, Z]	[y + 1/2, 1/2, z + 1/2]	[38]
39	[-Y, X, -Z]	[-y + 1/2, 1/2, 1/2 - z]	[39]
40	[Y, -X, -Z]	[y + 1/2, 1/2, 1/2 - z]	[40]
41	[-X, -Z, Y]	[-1/2, 1/2 - z, y + 1/2]	[41]
42	[X, -Z, -Y]	[1/2, 1/2 - z, 1/2 - y]	[42]
43	[X, Z, Y]	[1/2, z + 1/2, y + 1/2]	[43]
44	[-X, Z, -Y]	[-1/2, z + 1/2, 1/2 - y]	[44]
45	[-Z, -Y, X]	[-1/2 - z, 1/2 - y, 1/2]	[45]
46	[-Z, Y, -X]	[-1/2 - z, y + 1/2, 1/2]	[46]
47	[Z, -Y, -X]	[z + 1/2, 1/2 - y, 1/2]	[47]
48	[Z, Y, X]	[z + 1/2, y + 1/2, 1/2]	[48]

* Wyckoff site: 481, site symmetry: 1

Table 55: Wyckoff bond: 48a@481

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]
25	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[25]
26	$[X, Y, -Z]$	$[x, y, -z]$	[26]
27	$[X, -Y, Z]$	$[x, -y, z]$	[27]
28	$[-X, Y, Z]$	$[-x, y, z]$	[28]
29	$[-Z, -X, -Y]$	$[-z, -x, -y]$	[29]
30	$[-Z, X, Y]$	$[-z, x, y]$	[30]
31	$[Z, X, -Y]$	$[z, x, -y]$	[31]
32	$[Z, -X, Y]$	$[z, -x, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -z, -x]$	[33]
34	$[Y, -Z, X]$	$[y, -z, x]$	[34]
35	$[-Y, Z, X]$	$[-y, z, x]$	[35]
36	$[Y, Z, -X]$	$[y, z, -x]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[39]
40	$[Y, -X, -Z]$	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[46]

continued ...

Table 55

No.	vector	center	mapping
47	$[Z, -Y, -X]$	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[47]
48	$[Z, Y, X]$	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[48]