

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: $-4m.2$

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	$[X, Y, -X]$	$[\frac{1}{2}, \frac{1}{4}, 0]$	$[31, -37]$
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	$[0, Y, X]$	$[0, \frac{1}{2}, \frac{3}{4}]$	$[23, 48]$
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: **48g06c**

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: $-4m.2$

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: **24e06d**

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: **24f06d**

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: 48d08e

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: $\text{mm}2..$

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: $\text{mm}2..$

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: $\dots 2$

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	$[Y, X, -Z]$	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - z]$	[14]
15	$[Y, -X, Z]$	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[15]
16	$[-Y, X, Z]$	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	[16]
17	$[X, Z, -Y]$	$[\frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[19]
20	$[X, -Z, Y]$	$[\frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[20]
21	$[Z, Y, -X]$	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[21]
22	$[Z, -Y, X]$	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2}]$	[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	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - z]$	[39]
40	$[Y, -X, -Z]$	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[42]
43	$[X, Z, Y]$	$[\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2}]$	[46]
47	$[Z, -Y, -X]$	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[47]
48	$[Z, Y, X]$	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[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]