

SG No. 224 O_h^4 $Pn\bar{3}m$ [cubic]

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

* Wyckoff site: **2a**, site symmetry: $-43m$

Table 1: Wyckoff bond: **6a@2a**

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

Table 2: Wyckoff bond: **8b@2a**

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

Table 3: Wyckoff bond: **12c@2a**

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

Table 4: Wyckoff bond: 24d@2a

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

Table 5: Wyckoff bond: 24e@2a

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, -2]$
2	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[3, -4]$
3	$[0, X, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[5, -6]$
4	$[0, -X, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[7, -8]$
5	$[Y, 0, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[9, -10]$
6	$[Y, 0, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[11, -12]$
7	$[Y, X, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[13, -14]$
8	$[Y, -X, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[15, -16]$
9	$[X, 0, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[17, -18]$
10	$[-X, 0, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[19, -20]$
11	$[0, Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[21, -22]$
12	$[0, Y, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[23, -24]$
13	$[-X, -Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[25, -26]$
14	$[X, -Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[27, -28]$
15	$[0, -X, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[29, -30]$

continued ...

Table 5

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

Table 6: Wyckoff bond: 48f@2a

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[2]
3	$[-X, Y, -Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[3]
4	$[X, -Y, -Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[4]
5	$[Z, X, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[5]
6	$[Z, -X, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[6]
7	$[-Z, -X, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[7]
8	$[-Z, X, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[8]
9	$[Y, Z, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[9]
10	$[-Y, Z, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[10]
11	$[Y, -Z, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[12]
13	$[Y, X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[14]
15	$[Y, -X, Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[15]
16	$[-Y, X, Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[16]
17	$[X, Z, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[17]
18	$[-X, Z, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[19]
20	$[X, -Z, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[20]
21	$[Z, Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[21]
22	$[Z, -Y, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[22]
23	$[-Z, Y, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25]
26	$[X, Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[26]
27	$[X, -Y, Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[27]
28	$[-X, Y, Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[29]
30	$[-Z, X, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[30]
31	$[Z, X, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[31]

continued ...

Table 6

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

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

Table 7: Wyckoff bond: 4a@4b

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

Table 8: Wyckoff bond: 12b@4b

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

continued ...

Table 8

No.	vector	center	mapping
12	$[-X, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[12, -17, -36, 41]$

Table 9: Wyckoff bond: 12c@4b

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

Table 10: Wyckoff bond: 24d@4b

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

continued ...

Table 10

No.	vector	center	mapping
22	$[Z, -Y, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[22,-46]
23	$[-Z, Y, X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[23,-47]
24	$[-Z, -Y, -X]$	$[0, 0, 0]$	[24,-48]

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

Table 11: Wyckoff bond: 4a@4c

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

Table 12: Wyckoff bond: 12b@4c

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

Table 13: Wyckoff bond: 12c@4c

No.	vector	center	mapping
1	$[X, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1,14,-25,-38]
2	$[-X, X, 0]$	$[0, 0, \frac{1}{2}]$	[2,13,-26,-37]
3	$[-X, -X, 0]$	$[0, \frac{1}{2}, 0]$	[3,15,-27,-39]
4	$[X, X, 0]$	$[\frac{1}{2}, 0, 0]$	[4,16,-28,-40]
5	$[0, X, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[5,24,-29,-48]
6	$[0, -X, X]$	$[\frac{1}{2}, 0, 0]$	[6,23,-30,-47]
7	$[0, -X, -X]$	$[0, 0, \frac{1}{2}]$	[7,21,-31,-45]

continued ...

Table 13

No.	vector	center	mapping
8	$[0, X, X]$	$[0, \frac{1}{2}, 0]$	$[8, 22, -32, -46]$
9	$[-X, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[9, 19, -33, -43]$
10	$[X, 0, -X]$	$[0, \frac{1}{2}, 0]$	$[10, 20, -34, -44]$
11	$[-X, 0, -X]$	$[\frac{1}{2}, 0, 0]$	$[11, 18, -35, -42]$
12	$[X, 0, X]$	$[0, 0, \frac{1}{2}]$	$[12, 17, -36, -41]$

Table 14: Wyckoff bond: 24d@4c

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

* Wyckoff site: 6d, site symmetry: $-42.m$

Table 15: Wyckoff bond: 6a@6d

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[1, -2, -3, 4, -41, 42, 43, -44]$
2	$[0, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[5, -6, -7, 8, -37, 38, 39, -40]$
3	$[0, 0, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	$[9, -10, -11, 12, 45, -46, -47, 48]$

continued ...

Table 15

No.	vector	center	mapping
4	$[0, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[13, -14, -15, 16, -29, 30, 31, -32]$
5	$[X, 0, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[17, -18, -19, 20, -25, 26, 27, -28]$
6	$[0, 0, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[21, -22, -23, 24, 33, -34, -35, 36]$

Table 16: Wyckoff bond: 12b@6d

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

Table 17: Wyckoff bond: 12c@6d

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

Table 18: Wyckoff bond: 24d@6d

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

Table 19: Wyckoff bond: 24e@6d

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[1, -2]$
2	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[3, -4]$
3	$[0, X, Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[5, -6]$
4	$[0, -X, Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[7, -8]$
5	$[Y, 0, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	$[9, -10]$
6	$[Y, 0, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	$[11, -12]$
7	$[Y, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[13, -14]$
8	$[Y, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[15, -16]$
9	$[X, 0, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[17, -18]$
10	$[-X, 0, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[19, -20]$
11	$[0, Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[21, -22]$
12	$[0, Y, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[23, -24]$
13	$[-X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[25, -26]$
14	$[X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[27, -28]$
15	$[0, -X, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[29, -30]$

continued ...

Table 19

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

Table 20: Wyckoff bond: 24f06d

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

Table 21: Wyckoff bond: 48g@6d

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

continued ...

Table 21

No.	vector	center	mapping
47	$[Z, -Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[47]
48	$[Z, Y, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[48]

* Wyckoff site: 8e, site symmetry: .3m

Table 22: Wyckoff bond: 8a@8e

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

Table 23: Wyckoff bond: 24b@8e

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

continued ...

Table 23

No.	vector	center	mapping
23	$[-Y, X, X]$	$[-x, x + \frac{1}{2}, x + \frac{1}{2}]$	[23,30]
24	$[-Y, -X, -X]$	$[-x, -x, -x]$	[24,29]

Table 24: Wyckoff bond: 24c@8e

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

Table 25: Wyckoff bond: 48d@8e

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

continued ...

Table 25

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

* Wyckoff site: 12f, site symmetry: 2.22

Table 26: Wyckoff bond: 12a@12f

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

Table 27: Wyckoff bond: 12b@12f

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

Table 28: Wyckoff bond: 12c@12f

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

continued ...

Table 28

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

Table 29: Wyckoff bond: 24d@12f

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

Table 30: Wyckoff bond: 24e@12f

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

continued ...

Table 30

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

Table 31: Wyckoff bond: 24f@12f

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

continued ...

Table 31

No.	vector	center	mapping
24	$[-Y, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, 0]$	[46, -47]

Table 32: Wyckoff bond: 48g@12f

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

continued ...

Table 32

No.	vector	center	mapping
40	$[Y, -X, -Z]$	$[\frac{1}{4}, 0, \frac{3}{4}]$	[40]
41	$[-X, -Z, Y]$	$[0, \frac{3}{4}, \frac{1}{4}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[42]
43	$[X, Z, Y]$	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[43]
44	$[-X, Z, -Y]$	$[0, \frac{3}{4}, \frac{1}{4}]$	[44]
45	$[-Z, -Y, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{3}{4}, \frac{1}{4}, 0]$	[46]
47	$[Z, -Y, -X]$	$[\frac{3}{4}, \frac{1}{4}, 0]$	[47]
48	$[Z, Y, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[48]

* Wyckoff site: 12g, site symmetry: 2.mm

Table 33: Wyckoff bond: 12a@12g

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

Table 34: Wyckoff bond: 12b@12g

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

continued ...

Table 34

No.	vector	center	mapping
12	$[0, 0, X]$	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	$[22, 23, 34, 35]$

Table 35: Wyckoff bond: 24c@12g

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

Table 36: Wyckoff bond: 24d@12g

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

continued ...

Table 36

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

Table 37: Wyckoff bond: 48e@12g

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[2]
3	$[-X, Y, -Z]$	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[3]
4	$[X, -Y, -Z]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[4]
5	$[Z, X, Y]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[5]
6	$[Z, -X, -Y]$	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[6]
7	$[-Z, -X, Y]$	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[7]
8	$[-Z, X, -Y]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[8]
9	$[Y, Z, X]$	$[\frac{1}{4}, \frac{1}{4}, x]$	[9]
10	$[-Y, Z, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[10]
11	$[Y, -Z, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{4}, \frac{1}{4}, x]$	[12]
13	$[Y, X, -Z]$	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{3}{4}, -x, \frac{3}{4}]$	[14]
15	$[Y, -X, Z]$	$[\frac{3}{4}, -x, \frac{3}{4}]$	[15]
16	$[-Y, X, Z]$	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[16]
17	$[X, Z, -Y]$	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[17]
18	$[-X, Z, Y]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[18]
19	$[-X, -Z, -Y]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[19]
20	$[X, -Z, Y]$	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[20]
21	$[Z, Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, -x]$	[21]
22	$[Z, -Y, X]$	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[22]
23	$[-Z, Y, X]$	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, -x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[25]

continued ...

Table 37

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

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

Table 38: Wyckoff bond: 24a@24h

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, \frac{1}{4}, \frac{3}{4}]$	[1, -4]
2	$[0, -X, Y]$	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[2, -3]
3	$[Y, 0, X]$	$[\frac{3}{4}, x, \frac{1}{4}]$	[5, -8]
4	$[Y, 0, -X]$	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[6, -7]
5	$[X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, x]$	[9, -12]
6	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[10, -11]
7	$[X, 0, -Y]$	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[13, -16]
8	$[-X, 0, -Y]$	$[\frac{3}{4}, -x, \frac{1}{4}]$	[14, -15]
9	$[0, Y, -X]$	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[17, -20]
10	$[0, Y, X]$	$[-x, \frac{1}{4}, \frac{3}{4}]$	[18, -19]
11	$[Y, X, 0]$	$[\frac{1}{4}, \frac{3}{4}, -x]$	[21, -24]
12	$[Y, -X, 0]$	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[22, -23]
13	$[0, -X, -Y]$	$[-x, \frac{3}{4}, \frac{1}{4}]$	[25, -28]
14	$[0, X, -Y]$	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[26, -27]
15	$[-Y, 0, -X]$	$[\frac{1}{4}, -x, \frac{3}{4}]$	[29, -32]
16	$[-Y, 0, X]$	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[30, -31]

continued ...

Table 38

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

Table 39: Wyckoff bond: 24b@24h

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

Table 40: Wyckoff bond: 48c@24h

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

continued ...

Table 40

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

Table 41: Wyckoff bond: 24a@24i

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

Table 42: Wyckoff bond: 24b@24i

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

continued ...

Table 42

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

Table 43: Wyckoff bond: 48c@24i

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, y, y + \frac{1}{2}]$	[1]
2	$[-X, -Y, Z]$	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	[2]
3	$[-X, Y, -Z]$	$[0, y, -y]$	[3]
4	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2} - y, -y]$	[4]
5	$[Z, X, Y]$	$[y + \frac{1}{2}, \frac{1}{2}, y]$	[5]
6	$[Z, -X, -Y]$	$[y + \frac{1}{2}, 0, \frac{1}{2} - y]$	[6]
7	$[-Z, -X, Y]$	$[-y, 0, y]$	[7]
8	$[-Z, X, -Y]$	$[-y, \frac{1}{2}, \frac{1}{2} - y]$	[8]
9	$[Y, Z, X]$	$[y, y + \frac{1}{2}, \frac{1}{2}]$	[9]
10	$[-Y, Z, -X]$	$[\frac{1}{2} - y, y + \frac{1}{2}, 0]$	[10]
11	$[Y, -Z, -X]$	$[y, -y, 0]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{2} - y, -y, \frac{1}{2}]$	[12]
13	$[Y, X, -Z]$	$[y + \frac{1}{2}, 0, \frac{1}{2} - y]$	[13]
14	$[-Y, -X, -Z]$	$[-y, \frac{1}{2}, \frac{1}{2} - y]$	[14]
15	$[Y, -X, Z]$	$[y + \frac{1}{2}, \frac{1}{2}, y]$	[15]
16	$[-Y, X, Z]$	$[-y, 0, y]$	[16]
17	$[X, Z, -Y]$	$[0, y, -y]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{2}, y, y + \frac{1}{2}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{2}, \frac{1}{2} - y, -y]$	[19]
20	$[X, -Z, Y]$	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	[20]
21	$[Z, Y, -X]$	$[y, y + \frac{1}{2}, \frac{1}{2}]$	[21]
22	$[Z, -Y, X]$	$[y, -y, 0]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{2} - y, y + \frac{1}{2}, 0]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{2} - y, -y, \frac{1}{2}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{1}{2}, -y, \frac{1}{2} - y]$	[25]
26	$[X, Y, -Z]$	$[0, y + \frac{1}{2}, \frac{1}{2} - y]$	[26]
27	$[X, -Y, Z]$	$[0, -y, y]$	[27]
28	$[-X, Y, Z]$	$[\frac{1}{2}, y + \frac{1}{2}, y]$	[28]

continued ...

Table 43

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

* Wyckoff site: 24j, site symmetry: $\dots 2$

Table 44: Wyckoff bond: 24a@24j

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

continued ...

Table 44

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

Table 45: Wyckoff bond: 24b@24j

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

Table 46: Wyckoff bond: 48c@24j

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, y, -y]$	$[1]$
2	$[-X, -Y, Z]$	$[0, \frac{1}{2} - y, -y]$	$[2]$
3	$[-X, Y, -Z]$	$[0, y, y + \frac{1}{2}]$	$[3]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	$[4]$
5	$[Z, X, Y]$	$[-y, \frac{1}{2}, y]$	$[5]$

continued ...

Table 46

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

* Wyckoff site: 24k, site symmetry: $\dots m$

Table 47: Wyckoff bond: 24a@24k

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

Table 48: Wyckoff bond: 24b@24k

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, z]$	$[1, -38]$
2	$[-X, X, 0]$	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	$[2, -37]$
3	$[-X, -X, 0]$	$[\frac{1}{2} - x, x, \frac{1}{2} - z]$	$[3, -39]$
4	$[X, X, 0]$	$[x, \frac{1}{2} - x, \frac{1}{2} - z]$	$[4, -40]$
5	$[0, X, -X]$	$[z, x, x]$	$[5, -48]$
6	$[0, -X, X]$	$[z, \frac{1}{2} - x, \frac{1}{2} - x]$	$[6, -47]$
7	$[0, -X, -X]$	$[\frac{1}{2} - z, \frac{1}{2} - x, x]$	$[7, -45]$
8	$[0, X, X]$	$[\frac{1}{2} - z, x, \frac{1}{2} - x]$	$[8, -46]$
9	$[-X, 0, X]$	$[x, z, x]$	$[9, -43]$
10	$[X, 0, -X]$	$[\frac{1}{2} - x, z, \frac{1}{2} - x]$	$[10, -44]$
11	$[-X, 0, -X]$	$[x, \frac{1}{2} - z, \frac{1}{2} - x]$	$[11, -42]$
12	$[X, 0, X]$	$[\frac{1}{2} - x, \frac{1}{2} - z, x]$	$[12, -41]$
13	$[-X, X, 0]$	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	$[13, -26]$
14	$[X, -X, 0]$	$[-x, -x, -z]$	$[14, -25]$
15	$[-X, -X, 0]$	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	$[15, -27]$

continued ...

Table 48

No.	vector	center	mapping
16	$[X, X, 0]$	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[16, -28]
17	$[X, 0, X]$	$[x + \frac{1}{2}, z + \frac{1}{2}, -x]$	[17, -36]
18	$[-X, 0, -X]$	$[-x, z + \frac{1}{2}, x + \frac{1}{2}]$	[18, -35]
19	$[-X, 0, X]$	$[-x, -z, -x]$	[19, -33]
20	$[X, 0, -X]$	$[x + \frac{1}{2}, -z, x + \frac{1}{2}]$	[20, -34]
21	$[0, -X, -X]$	$[z + \frac{1}{2}, x + \frac{1}{2}, -x]$	[21, -31]
22	$[0, X, X]$	$[z + \frac{1}{2}, -x, x + \frac{1}{2}]$	[22, -32]
23	$[0, -X, X]$	$[-z, x + \frac{1}{2}, x + \frac{1}{2}]$	[23, -30]
24	$[0, X, -X]$	$[-z, -x, -x]$	[24, -29]

Table 49: Wyckoff bond: 48c@24k

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	[2]
3	$[-X, Y, -Z]$	$[\frac{1}{2} - x, x, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[x, \frac{1}{2} - x, \frac{1}{2} - z]$	[4]
5	$[Z, X, Y]$	$[z, x, x]$	[5]
6	$[Z, -X, -Y]$	$[z, \frac{1}{2} - x, \frac{1}{2} - x]$	[6]
7	$[-Z, -X, Y]$	$[\frac{1}{2} - z, \frac{1}{2} - x, x]$	[7]
8	$[-Z, X, -Y]$	$[\frac{1}{2} - z, x, \frac{1}{2} - x]$	[8]
9	$[Y, Z, X]$	$[x, z, x]$	[9]
10	$[-Y, Z, -X]$	$[\frac{1}{2} - x, z, \frac{1}{2} - x]$	[10]
11	$[Y, -Z, -X]$	$[x, \frac{1}{2} - z, \frac{1}{2} - x]$	[11]
12	$[-Y, -Z, X]$	$[\frac{1}{2} - x, \frac{1}{2} - z, x]$	[12]
13	$[Y, X, -Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	[13]
14	$[-Y, -X, -Z]$	$[-x, -x, -z]$	[14]
15	$[Y, -X, Z]$	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	[15]
16	$[-Y, X, Z]$	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[16]
17	$[X, Z, -Y]$	$[x + \frac{1}{2}, z + \frac{1}{2}, -x]$	[17]
18	$[-X, Z, Y]$	$[-x, z + \frac{1}{2}, x + \frac{1}{2}]$	[18]
19	$[-X, -Z, -Y]$	$[-x, -z, -x]$	[19]
20	$[X, -Z, Y]$	$[x + \frac{1}{2}, -z, x + \frac{1}{2}]$	[20]
21	$[Z, Y, -X]$	$[z + \frac{1}{2}, x + \frac{1}{2}, -x]$	[21]
22	$[Z, -Y, X]$	$[z + \frac{1}{2}, -x, x + \frac{1}{2}]$	[22]
23	$[-Z, Y, X]$	$[-z, x + \frac{1}{2}, x + \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[-z, -x, -x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, -x, -z]$	[25]
26	$[X, Y, -Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	[26]
27	$[X, -Y, Z]$	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	[27]
28	$[-X, Y, Z]$	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[28]
29	$[-Z, -X, -Y]$	$[-z, -x, -x]$	[29]
30	$[-Z, X, Y]$	$[-z, x + \frac{1}{2}, x + \frac{1}{2}]$	[30]
31	$[Z, X, -Y]$	$[z + \frac{1}{2}, x + \frac{1}{2}, -x]$	[31]

continued ...

Table 49

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

* Wyckoff site: 481, site symmetry: 1

Table 50: Wyckoff bond: 48a@481

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

continued ...

Table 50

No.	vector	center	mapping
23	$[-Z, Y, X]$	$[-z, y + \frac{1}{2}, x + \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[-z, -y, -x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[25]
26	$[X, Y, -Z]$	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[26]
27	$[X, -Y, Z]$	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[27]
28	$[-X, Y, Z]$	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[28]
29	$[-Z, -X, -Y]$	$[-z, -x, -y]$	[29]
30	$[-Z, X, Y]$	$[-z, x + \frac{1}{2}, y + \frac{1}{2}]$	[30]
31	$[Z, X, -Y]$	$[z + \frac{1}{2}, x + \frac{1}{2}, -y]$	[31]
32	$[Z, -X, Y]$	$[z + \frac{1}{2}, -x, y + \frac{1}{2}]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -z, -x]$	[33]
34	$[Y, -Z, X]$	$[y + \frac{1}{2}, -z, x + \frac{1}{2}]$	[34]
35	$[-Y, Z, X]$	$[-y, z + \frac{1}{2}, x + \frac{1}{2}]$	[35]
36	$[Y, Z, -X]$	$[y + \frac{1}{2}, z + \frac{1}{2}, -x]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[37]
38	$[Y, X, Z]$	$[y, x, z]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2} - y, x, \frac{1}{2} - z]$	[39]
40	$[Y, -X, -Z]$	$[y, \frac{1}{2} - x, \frac{1}{2} - z]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2} - x, \frac{1}{2} - z, y]$	[41]
42	$[X, -Z, -Y]$	$[x, \frac{1}{2} - z, \frac{1}{2} - y]$	[42]
43	$[X, Z, Y]$	$[x, z, y]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2} - x, z, \frac{1}{2} - y]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, x]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2} - z, y, \frac{1}{2} - x]$	[46]
47	$[Z, -Y, -X]$	$[z, \frac{1}{2} - y, \frac{1}{2} - x]$	[47]
48	$[Z, Y, X]$	$[z, y, x]$	[48]