

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: .-3m

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: .-3m

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]	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[13, -14, -15, 16, -29, 30, 31, -32]
5	[X, 0, 0]	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[17, -18, -19, 20, -25, 26, 27, -28]
6	[0, 0, -X]	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[21, -22, -23, 24, 33, -34, -35, 36]

Table 16: Wyckoff bond: 12b@6d

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

Table 17: Wyckoff bond: 12c@6d

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

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	$[Z, -Y, -X]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[47]
48	$[Z, Y, X]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[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	$[-X, -X, X]$	$\left[\frac{1}{2} - x, \frac{1}{2} - x, x\right]$	[2, 7, 12, 37, 41, 45]
3	$[-X, X, -X]$	$\left[\frac{1}{2} - x, x, \frac{1}{2} - x\right]$	[3, 8, 10, 39, 44, 46]
4	$[X, -X, -X]$	$\left[x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[4, 6, 11, 40, 42, 47]
5	$[X, X, -X]$	$\left[x + \frac{1}{2}, x + \frac{1}{2}, -x\right]$	[13, 17, 21, 26, 31, 36]
6	$[-X, -X, -X]$	$[-x, -x, -x]$	[14, 19, 24, 25, 29, 33]
7	$[X, -X, X]$	$\left[x + \frac{1}{2}, -x, x + \frac{1}{2}\right]$	[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	$[-X, -X, Y]$	$\left[\frac{1}{2} - x, \frac{1}{2} - x, x\right]$	[2, 37]
3	$[-X, X, -Y]$	$\left[\frac{1}{2} - x, x, \frac{1}{2} - x\right]$	[3, 39]
4	$[X, -X, -Y]$	$\left[x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[4, 40]
5	$[Y, X, X]$	$[x, x, x]$	[5, 48]
6	$[Y, -X, -X]$	$\left[x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[6, 47]
7	$[-Y, -X, X]$	$\left[\frac{1}{2} - x, \frac{1}{2} - x, x\right]$	[7, 45]
8	$[-Y, X, -X]$	$\left[\frac{1}{2} - x, x, \frac{1}{2} - x\right]$	[8, 46]
9	$[X, Y, X]$	$[x, x, x]$	[9, 43]
10	$[-X, Y, -X]$	$\left[\frac{1}{2} - x, x, \frac{1}{2} - x\right]$	[10, 44]
11	$[X, -Y, -X]$	$\left[x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[11, 42]
12	$[-X, -Y, X]$	$\left[\frac{1}{2} - x, \frac{1}{2} - x, x\right]$	[12, 41]
13	$[X, X, -Y]$	$\left[x + \frac{1}{2}, x + \frac{1}{2}, -x\right]$	[13, 26]
14	$[-X, -X, -Y]$	$[-x, -x, -x]$	[14, 25]
15	$[X, -X, Y]$	$\left[x + \frac{1}{2}, -x, x + \frac{1}{2}\right]$	[15, 27]
16	$[-X, X, Y]$	$[-x, x + \frac{1}{2}, x + \frac{1}{2}]$	[16, 28]
17	$[X, Y, -X]$	$\left[x + \frac{1}{2}, x + \frac{1}{2}, -x\right]$	[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	$[X, -Y, X]$	$\left[x + \frac{1}{2}, -x, x + \frac{1}{2}\right]$	[20, 34]
21	$[Y, X, -X]$	$\left[x + \frac{1}{2}, x + \frac{1}{2}, -x\right]$	[21, 31]
22	$[Y, -X, X]$	$\left[x + \frac{1}{2}, -x, x + \frac{1}{2}\right]$	[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	$[-Y, X, 0]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[46, -47]

Table 32: Wyckoff bond: 48g@12f

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

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

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: ..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: . . 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]