

SG No. 222 $O_h^2 Pn\bar{3}n$ [cubic]

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

* Wyckoff site: 2a, site symmetry: 432

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, 17, -18, -19, 20]
2	[0, X, 0]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[5, -6, -7, 8, 13, -14, -15, 16]
3	[0, 0, X]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[9, -10, -11, 12, -21, 22, 23, -24]
4	[-X, 0, 0]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25, -26, -27, 28, 41, -42, -43, 44]
5	[0, -X, 0]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[29, -30, -31, 32, 37, -38, -39, 40]
6	[0, 0, -X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[33, -34, -35, 36, -45, 46, 47, -48]

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, -14, -19, -24]
2	[-X, -X, X]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[2, 7, 12, -13, -17, -21]
3	[-X, X, -X]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[3, 8, 10, -15, -20, -22]
4	[X, -X, -X]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[4, 6, 11, -16, -18, -23]
5	[-X, -X, -X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25, 29, 33, -38, -43, -48]
6	[X, X, -X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[26, 31, 36, -37, -41, -45]
7	[X, -X, X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[27, 32, 34, -39, -44, -46]
8	[-X, X, X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[28, 30, 35, -40, -42, -47]

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, 13, -14]
2	[-X, X, 0]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[3, -4, -15, 16]
3	[0, X, X]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[5, -6, 23, -24]
4	[0, -X, X]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[7, -8, -21, 22]
5	[X, 0, X]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[9, -10, -19, 20]
6	[X, 0, -X]	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[11, -12, 17, -18]
7	[-X, -X, 0]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25, -26, 37, -38]
8	[X, -X, 0]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[27, -28, -39, 40]
9	[0, -X, -X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[29, -30, 47, -48]
10	[0, X, -X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[31, -32, -45, 46]
11	[-X, 0, -X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[33, -34, -43, 44]
12	[-X, 0, X]	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[35, -36, 41, -42]

Table 4: Wyckoff bond: 24d@2a

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

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	$[Y, X, 0]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[13, -14]
8	$[Y, -X, 0]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[15, -16]
9	$[X, 0, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[17, -18]
10	$[-X, 0, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[19, -20]
11	$[0, Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[21, -22]
12	$[0, Y, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[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	$[-Y, -X, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[37,-38]
20	$[-Y, X, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[39,-40]
21	$[-X, 0, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[41,-42]
22	$[X, 0, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[43,-44]
23	$[0, -Y, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[45,-46]
24	$[0, -Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[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	$[Y, X, -Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[14]
15	$[Y, -X, Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[15]
16	$[-Y, X, Z]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[16]
17	$[X, Z, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[19]
20	$[X, -Z, Y]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[20]
21	$[Z, Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[21]
22	$[Z, -Y, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25]
26	$[X, Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[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	$[-Y, -X, Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[37]
38	$[Y, X, Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[39]
40	$[Y, -X, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[40]
41	$[-X, -Z, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[42]
43	$[X, Z, Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[44]
45	$[-Z, -Y, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[46]
47	$[Z, -Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[47]
48	$[Z, Y, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[48]

* Wyckoff site: 6b, site symmetry: 42.2

Table 7: Wyckoff bond: 6a@6b

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

Table 8: Wyckoff bond: 12b@6b

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

continued ...

Table 8

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

Table 9: Wyckoff bond: 12c@6b

No.	vector	center	mapping
1	$[0, 0, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, 2, -3, -4]$
2	$[X, 0, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[5, 6, -7, -8]$
3	$[0, X, 0]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[9, 10, -11, -12]$
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	$[0, 0, -X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[25, 26, -27, -28]$
8	$[-X, 0, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[29, 30, -31, -32]$
9	$[0, -X, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	$[33, 34, -35, -36]$
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 10: Wyckoff bond: 24d@6b

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

continued ...

Table 10

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

Table 11: Wyckoff bond: 24e06b

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[1, -2]
2	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[3, -4]
3	$[0, X, Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[5, -6]
4	$[0, -X, Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[7, -8]
5	$[Y, 0, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[9, -10]
6	$[Y, 0, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[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	$[-X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[25, -26]
14	$[X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[27, -28]
15	$[0, -X, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[29, -30]
16	$[0, X, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[31, -32]
17	$[-Y, 0, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[33, -34]
18	$[-Y, 0, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[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 12: Wyckoff bond: 24f06b

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

continued ...

Table 12

No.	vector	center	mapping
6	$[-X, Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[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	$[0, -X, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[25, -28]
14	$[0, X, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[26, -27]
15	$[-Y, 0, -X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[29, -32]
16	$[-Y, 0, X]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[30, -31]
17	$[-X, -Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[33, -36]
18	$[X, -Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[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 13: Wyckoff bond: 48g@6b

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

continued ...

Table 13

No.	vector	center	mapping
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	$[-X, -Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[27]
28	$[-X, Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[29]
30	$[-Z, X, Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[30]
31	$[Z, X, -Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[31]
32	$[Z, -X, Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[32]
33	$[-Y, -Z, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[33]
34	$[Y, -Z, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[34]
35	$[-Y, Z, X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[35]
36	$[Y, Z, -X]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[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]
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: 8c, site symmetry: $\bar{3}$.

Table 14: Wyckoff bond: 8a@8c

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

Table 15: Wyckoff bond: 24b@8c

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	$[Y, X, -Z]$	$[0, 0, \frac{1}{2}]$	$[13, -37]$
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: 12d, site symmetry: -4 .

Table 16: Wyckoff bond: 12a@12d

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

Table 17: Wyckoff bond: 24b@12d

No.	vector	center	mapping
1	$[0, X, Y]$	$[0, \frac{3}{4}, \frac{1}{4}]$	[1,-4]
2	$[0, -X, Y]$	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[2,-3]
3	$[Y, 0, X]$	$[\frac{1}{4}, 0, \frac{3}{4}]$	[5,-8]
4	$[Y, 0, -X]$	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	[6,-7]
5	$[X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, 0]$	[9,-12]
6	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[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	$[0, -X, -Y]$	$[0, \frac{1}{4}, \frac{3}{4}]$	[25,-28]
14	$[0, X, -Y]$	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[26,-27]
15	$[-Y, 0, -X]$	$[\frac{3}{4}, 0, \frac{1}{4}]$	[29,-32]
16	$[-Y, 0, X]$	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[30,-31]
17	$[-X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, 0]$	[33,-36]
18	$[X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[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]
24	$[-Y, X, 0]$	$[\frac{3}{4}, \frac{1}{4}, 0]$	[46,-47]

Table 18: Wyckoff bond: 48c@12d

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

continued ...

Table 18

No.	vector	center	mapping
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	$[-X, -Y, -Z]$	$[0, \frac{1}{4}, \frac{3}{4}]$	[25]
26	$[X, Y, -Z]$	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[26]
27	$[X, -Y, Z]$	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[27]
28	$[-X, Y, Z]$	$[0, \frac{1}{4}, \frac{3}{4}]$	[28]
29	$[-Z, -X, -Y]$	$[\frac{3}{4}, 0, \frac{1}{4}]$	[29]
30	$[-Z, X, Y]$	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[30]
31	$[Z, X, -Y]$	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[31]
32	$[Z, -X, Y]$	$[\frac{3}{4}, 0, \frac{1}{4}]$	[32]
33	$[-Y, -Z, -X]$	$[\frac{1}{4}, \frac{3}{4}, 0]$	[33]
34	$[Y, -Z, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[34]
35	$[-Y, Z, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[35]
36	$[Y, Z, -X]$	$[\frac{1}{4}, \frac{3}{4}, 0]$	[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]
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: 12e, site symmetry: 4..

Table 19: Wyckoff bond: 12a@12e

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

continued ...

Table 19

No.	vector	center	mapping
7	$[-X, 0, 0]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[25, 28, 41, 44]
8	$[X, 0, 0]$	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[26, 27, 42, 43]
9	$[0, -X, 0]$	$[\frac{3}{4}, -x, \frac{3}{4}]$	[29, 32, 37, 40]
10	$[0, X, 0]$	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[30, 31, 38, 39]
11	$[0, 0, -X]$	$[\frac{3}{4}, \frac{3}{4}, -x]$	[33, 36, 46, 47]
12	$[0, 0, X]$	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[34, 35, 45, 48]

Table 20: Wyckoff bond: 24b@12e

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	$[X, 0, -Y]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[13, -16]
8	$[-X, 0, -Y]$	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[14, -15]
9	$[0, Y, -X]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[17, -20]
10	$[0, Y, X]$	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[18, -19]
11	$[Y, X, 0]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[21, -24]
12	$[Y, -X, 0]$	$[\frac{1}{4}, \frac{1}{4}, x]$	[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	$[-X, 0, Y]$	$[\frac{3}{4}, -x, \frac{3}{4}]$	[37, -40]
20	$[X, 0, Y]$	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[38, -39]
21	$[0, -Y, X]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[41, -44]
22	$[0, -Y, -X]$	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[42, -43]
23	$[-Y, -X, 0]$	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[45, -48]
24	$[-Y, X, 0]$	$[\frac{3}{4}, \frac{3}{4}, -x]$	[46, -47]

Table 21: Wyckoff bond: 48c@12e

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]

continued ...

Table 21

No.	vector	center	mapping
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	$[Y, X, -Z]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[14]
15	$[Y, -X, Z]$	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[15]
16	$[-Y, X, Z]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[16]
17	$[X, Z, -Y]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[19]
20	$[X, -Z, Y]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[20]
21	$[Z, Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[21]
22	$[Z, -Y, X]$	$[\frac{1}{4}, \frac{1}{4}, x]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{4}, \frac{1}{4}, x]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[25]
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	$[-Y, -X, Z]$	$[\frac{3}{4}, -x, \frac{3}{4}]$	[37]
38	$[Y, X, Z]$	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[39]
40	$[Y, -X, -Z]$	$[\frac{3}{4}, -x, \frac{3}{4}]$	[40]
41	$[-X, -Z, Y]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[43]
44	$[-X, Z, -Y]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[44]
45	$[-Z, -Y, X]$	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, -x]$	[46]
47	$[Z, -Y, -X]$	$[\frac{3}{4}, \frac{3}{4}, -x]$	[47]
48	$[Z, Y, X]$	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[48]

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

Table 22: Wyckoff bond: 16a@16f

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

Table 23: Wyckoff bond: 48b@16f

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

continued ...

Table 23

No.	vector	center	mapping
24	$[-Z, -Y, -X]$	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, -x, -x]$	[25]
26	$[X, Y, -Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, -x]$	[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	$[-Y, -X, Z]$	$[-x, -x, x + \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[-x, x + \frac{1}{2}, -x]$	[39]
40	$[Y, -X, -Z]$	$[x + \frac{1}{2}, -x, -x]$	[40]
41	$[-X, -Z, Y]$	$[-x, -x, x + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, -x, -x]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[-x, x + \frac{1}{2}, -x]$	[44]
45	$[-Z, -Y, X]$	$[-x, -x, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[-x, x + \frac{1}{2}, -x]$	[46]
47	$[Z, -Y, -X]$	$[x + \frac{1}{2}, -x, -x]$	[47]
48	$[Z, Y, X]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[48]

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

Table 24: Wyckoff bond: 24a@24g

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

continued ...

Table 24

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

Table 25: Wyckoff bond: 24b@24g

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

Table 26: Wyckoff bond: 48c@24g

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

continued ...

Table 26

No.	vector	center	mapping
47	$[Z, -Y, -X]$	$[\frac{3}{4}, \frac{1}{4}, -x]$	[47]
48	$[Z, Y, X]$	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[48]

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

Table 27: Wyckoff bond: 24a@24h

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

Table 28: Wyckoff bond: 24b@24h

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

continued ...

Table 28

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

Table 29: Wyckoff bond: 48c@24h

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

continued ...

Table 29

No.	vector	center	mapping
23	$[-Z, Y, X]$	$[\frac{1}{2} - y, y, \frac{1}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{4}]$	[24]
25	$[-X, -Y, -Z]$	$[\frac{3}{4}, -y, -y]$	[25]
26	$[X, Y, -Z]$	$[\frac{3}{4}, y + \frac{1}{2}, -y]$	[26]
27	$[X, -Y, Z]$	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[27]
28	$[-X, Y, Z]$	$[\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[28]
29	$[-Z, -X, -Y]$	$[-y, \frac{3}{4}, -y]$	[29]
30	$[-Z, X, Y]$	$[-y, \frac{3}{4}, y + \frac{1}{2}]$	[30]
31	$[Z, X, -Y]$	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[31]
32	$[Z, -X, Y]$	$[y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -y, \frac{3}{4}]$	[33]
34	$[Y, -Z, X]$	$[y + \frac{1}{2}, -y, \frac{3}{4}]$	[34]
35	$[-Y, Z, X]$	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[35]
36	$[Y, Z, -X]$	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[36]
37	$[-Y, -X, Z]$	$[-y, \frac{3}{4}, y + \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[-y, \frac{3}{4}, -y]$	[39]
40	$[Y, -X, -Z]$	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[40]
41	$[-X, -Z, Y]$	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{3}{4}, -y, -y]$	[42]
43	$[X, Z, Y]$	$[\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{3}{4}, y + \frac{1}{2}, -y]$	[44]
45	$[-Z, -Y, X]$	$[-y, -y, \frac{3}{4}]$	[45]
46	$[-Z, Y, -X]$	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[46]
47	$[Z, -Y, -X]$	$[y + \frac{1}{2}, -y, \frac{3}{4}]$	[47]
48	$[Z, Y, X]$	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[48]

* Wyckoff site: 48i, site symmetry: 1

Table 30: Wyckoff bond: 48a@48i

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	$[Y, X, -Z]$	$[y, x, \frac{1}{2} - z]$	[13]

continued ...

Table 30

No.	vector	center	mapping
14	$[-Y, -X, -Z]$	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[14]
15	$[Y, -X, Z]$	$[y, \frac{1}{2} - x, z]$	[15]
16	$[-Y, X, Z]$	$[\frac{1}{2} - y, x, z]$	[16]
17	$[X, Z, -Y]$	$[x, z, \frac{1}{2} - y]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{2} - x, z, y]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[19]
20	$[X, -Z, Y]$	$[x, \frac{1}{2} - z, y]$	[20]
21	$[Z, Y, -X]$	$[z, y, \frac{1}{2} - x]$	[21]
22	$[Z, -Y, X]$	$[z, \frac{1}{2} - y, x]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{2} - z, y, x]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[25]
26	$[X, Y, -Z]$	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[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	$[-Y, -X, Z]$	$[-y, -x, z + \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[-y, x + \frac{1}{2}, -z]$	[39]
40	$[Y, -X, -Z]$	$[y + \frac{1}{2}, -x, -z]$	[40]
41	$[-X, -Z, Y]$	$[-x, -z, y + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, -z, -y]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[-x, z + \frac{1}{2}, -y]$	[44]
45	$[-Z, -Y, X]$	$[-z, -y, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[-z, y + \frac{1}{2}, -x]$	[46]
47	$[Z, -Y, -X]$	$[z + \frac{1}{2}, -y, -x]$	[47]
48	$[Z, Y, X]$	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[48]