

SG No. 226  $O_h^6 Fm\bar{3}c$  [ cubic ]

\* plus set:  $+ [0, 0, 0], + [0, \frac{1}{2}, \frac{1}{2}], + [\frac{1}{2}, 0, \frac{1}{2}], + [\frac{1}{2}, \frac{1}{2}, 0]$

\* Wyckoff site: **8a**, site symmetry: **432**

Table 1: Wyckoff bond: 24a@8a

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: 32b@8a

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: 48c@8a

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: 96d@8a

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: 96e@8a

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: 192f08a

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: 8b, site symmetry:  $m-3$ .

Table 7: Wyckoff bond: 24a@8b

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

Table 8: Wyckoff bond: 32b@8b

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

Table 9: Wyckoff bond: 48c@8b

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

Table 10: Wyckoff bond: 96d@8b

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

\* Wyckoff site: 24c, site symmetry:  $-4m.2$

Table 11: Wyckoff bond: 24a@24c

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

Table 12: Wyckoff bond: 48b@24c

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

Table 13: Wyckoff bond: 48c@24c

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

Table 14: Wyckoff bond: 96d@24c

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

Table 15: Wyckoff bond: 96e@24c

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

*continued ...*

Table 15

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

Table 16: Wyckoff bond: 96f@24c

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



Table 17: Wyckoff bond: 192g@24c

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

continued ...

Table 17

No.	vector	center	mapping
47	$[Z, -Y, -X]$	$[0, 0, \frac{1}{4}]$	[47]
48	$[Z, Y, X]$	$[0, 0, \frac{3}{4}]$	[48]

\* Wyckoff site: 24d, site symmetry:  $4/m.$

Table 18: Wyckoff bond: 24a@24d

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

Table 19: Wyckoff bond: 48b@24d

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

Table 20: Wyckoff bond: 96c@24d

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

*continued ...*

Table 20

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

\* Wyckoff site: 48e, site symmetry:  $\text{mm}2..$

Table 21: Wyckoff bond: 48a@48e

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

Table 22: Wyckoff bond: 48b@48e

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

*continued ...*

Table 22

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

Table 23: Wyckoff bond: 96c@48e

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

Table 24: Wyckoff bond: 96d@48e

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

Table 25: Wyckoff bond: 192e@48e

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

*continued ...*

Table 25

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

\* Wyckoff site: **48f**, site symmetry: **4..**

Table 26: Wyckoff bond: **48a@48f**

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

*continued ...*

Table 26

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

Table 27: Wyckoff bond: 96b@48f

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

Table 28: Wyckoff bond: 192c@48f

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

continued ...

Table 28

No.	vector	center	mapping
5	$[Z, X, Y]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[5]
6	$[Z, -X, -Y]$	$[\frac{1}{4}, -x, \frac{3}{4}]$	[6]
7	$[-Z, -X, Y]$	$[\frac{1}{4}, -x, \frac{3}{4}]$	[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	$[-Y, Z, -X]$	$[\frac{3}{4}, \frac{1}{4}, -x]$	[10]
11	$[Y, -Z, -X]$	$[\frac{3}{4}, \frac{1}{4}, -x]$	[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	$[-Y, -X, -Z]$	$[\frac{1}{4}, -x, \frac{3}{4}]$	[14]
15	$[Y, -X, Z]$	$[\frac{1}{4}, -x, \frac{3}{4}]$	[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	$[-X, Z, Y]$	$[-x, \frac{3}{4}, \frac{1}{4}]$	[18]
19	$[-X, -Z, -Y]$	$[-x, \frac{3}{4}, \frac{1}{4}]$	[19]
20	$[X, -Z, Y]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[20]
21	$[Z, Y, -X]$	$[\frac{3}{4}, \frac{1}{4}, -x]$	[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	$[-Z, -Y, -X]$	$[\frac{3}{4}, \frac{1}{4}, -x]$	[24]
25	$[-X, -Y, -Z]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[25]
26	$[X, Y, -Z]$	$[x, \frac{1}{4}, \frac{3}{4}]$	[26]
27	$[X, -Y, Z]$	$[x, \frac{1}{4}, \frac{3}{4}]$	[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	$[-Z, X, Y]$	$[\frac{3}{4}, x, \frac{1}{4}]$	[30]
31	$[Z, X, -Y]$	$[\frac{3}{4}, x, \frac{1}{4}]$	[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	$[Y, -Z, X]$	$[\frac{1}{4}, \frac{3}{4}, x]$	[34]
35	$[-Y, Z, X]$	$[\frac{1}{4}, \frac{3}{4}, x]$	[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	$[Y, X, Z]$	$[\frac{3}{4}, x, \frac{1}{4}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{3}{4}, x, \frac{1}{4}]$	[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	$[X, -Z, -Y]$	$[x, \frac{1}{4}, \frac{3}{4}]$	[42]
43	$[X, Z, Y]$	$[x, \frac{1}{4}, \frac{3}{4}]$	[43]
44	$[-X, Z, -Y]$	$[-x, \frac{3}{4}, \frac{3}{4}]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{4}, \frac{3}{4}, x]$	[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	$[Z, Y, X]$	$[\frac{1}{4}, \frac{3}{4}, x]$	[48]

\* Wyckoff site: 64g, site symmetry: .3.



Table 29: Wyckoff bond: 64a@64g

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

Table 30: Wyckoff bond: 192b@64g

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

continued ...

Table 30

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	$[X, Y, -Z]$	$[x, x, -x]$	[26]
27	$[X, -Y, Z]$	$[x, -x, x]$	[27]
28	$[-X, Y, Z]$	$[-x, x, x]$	[28]
29	$[-Z, -X, -Y]$	$[-x, -x, -x]$	[29]
30	$[-Z, X, Y]$	$[-x, x, x]$	[30]
31	$[Z, X, -Y]$	$[x, x, -x]$	[31]
32	$[Z, -X, Y]$	$[x, -x, x]$	[32]
33	$[-Y, -Z, -X]$	$[-x, -x, -x]$	[33]
34	$[Y, -Z, X]$	$[x, -x, x]$	[34]
35	$[-Y, Z, X]$	$[-x, x, x]$	[35]
36	$[Y, Z, -X]$	$[x, x, -x]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[39]
40	$[Y, -X, -Z]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[42]
43	$[X, Z, Y]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[46]
47	$[Z, -Y, -X]$	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[47]
48	$[Z, Y, X]$	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[48]

\* Wyckoff site: 96h, site symmetry:  $\dots 2$

Table 31: Wyckoff bond: 96a@96h

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

*continued ...*

Table 31

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

Table 32: Wyckoff bond: 96b@96h

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

Table 33: Wyckoff bond: 192c@96h

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

continued ...

Table 33

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

\* Wyckoff site: 96i, site symmetry:  $m..$

Table 34: Wyckoff bond: 96a@96i

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

Table 35: Wyckoff bond: 96b@96i

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	[1,-28]
2	$[-X, 0, 0]$	$[0, -y, z]$	[2,-27]
3	$[-X, 0, 0]$	$[0, y, -z]$	[3,-26]
4	$[X, 0, 0]$	$[0, -y, -z]$	[4,-25]
5	$[0, X, 0]$	$[z, 0, y]$	[5,-32]
6	$[0, -X, 0]$	$[z, 0, -y]$	[6,-31]

*continued ...*

Table 35

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

Table 36: Wyckoff bond: 192c@96i

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

continued ...

Table 36

No.	vector	center	mapping
23	$[-Z, Y, X]$	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2}]$	[24]
25	$[-X, -Y, -Z]$	$[0, -y, -z]$	[25]
26	$[X, Y, -Z]$	$[0, y, -z]$	[26]
27	$[X, -Y, Z]$	$[0, -y, z]$	[27]
28	$[-X, Y, Z]$	$[0, y, z]$	[28]
29	$[-Z, -X, -Y]$	$[-z, 0, -y]$	[29]
30	$[-Z, X, Y]$	$[-z, 0, y]$	[30]
31	$[Z, X, -Y]$	$[z, 0, -y]$	[31]
32	$[Z, -X, Y]$	$[z, 0, y]$	[32]
33	$[-Y, -Z, -X]$	$[-y, -z, 0]$	[33]
34	$[Y, -Z, X]$	$[y, -z, 0]$	[34]
35	$[-Y, Z, X]$	$[-y, z, 0]$	[35]
36	$[Y, Z, -X]$	$[y, z, 0]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	[37]
38	$[Y, X, Z]$	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - z]$	[39]
40	$[Y, -X, -Z]$	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[42]
43	$[X, Z, Y]$	$[\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2}]$	[46]
47	$[Z, -Y, -X]$	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[47]
48	$[Z, Y, X]$	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[48]

\* Wyckoff site: 192j, site symmetry: 1

Table 37: Wyckoff bond: 192a@192j

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, -z]$	[4]
5	$[Z, X, Y]$	$[z, x, y]$	[5]
6	$[Z, -X, -Y]$	$[z, -x, -y]$	[6]
7	$[-Z, -X, Y]$	$[-z, -x, y]$	[7]
8	$[-Z, X, -Y]$	$[-z, x, -y]$	[8]
9	$[Y, Z, X]$	$[y, z, x]$	[9]
10	$[-Y, Z, -X]$	$[-y, z, -x]$	[10]
11	$[Y, -Z, -X]$	$[y, -z, -x]$	[11]
12	$[-Y, -Z, X]$	$[-y, -z, x]$	[12]
13	$[Y, X, -Z]$	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[13]

*continued ...*

Table 37

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