

SG No. 227 O_h^7 $Fd\bar{3}m$ [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: $-43m$

Table 1: Wyckoff bond: 24a@8a

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

Table 2: Wyckoff bond: 32b@8a

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

Table 3: Wyckoff bond: 48c@8a

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

Table 4: Wyckoff bond: 96d@8a

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

Table 5: Wyckoff bond: 96e@8a

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

continued ...

Table 5

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

Table 6: Wyckoff bond: 192f08a

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

continued ...

Table 6

No.	vector	center	mapping
32	$[Z, -X, Y]$	$[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}]$	[32]
33	$[-Y, -Z, -X]$	$[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}]$	[33]
34	$[Y, -Z, X]$	$[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}]$	[34]
35	$[-Y, Z, X]$	$[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}]$	[35]
36	$[Y, Z, -X]$	$[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}]$	[36]
37	$[-Y, -X, Z]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[37]
38	$[Y, X, Z]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[38]
39	$[-Y, X, -Z]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[39]
40	$[Y, -X, -Z]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[40]
41	$[-X, -Z, Y]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[41]
42	$[X, -Z, -Y]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[42]
43	$[X, Z, Y]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[43]
44	$[-X, Z, -Y]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[44]
45	$[-Z, -Y, X]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[45]
46	$[-Z, Y, -X]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[46]
47	$[Z, -Y, -X]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[47]
48	$[Z, Y, X]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[48]

* Wyckoff site: 8b, site symmetry: $-43m$

Table 7: Wyckoff bond: 24a@8b

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

Table 8: Wyckoff bond: 32b@8b

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

Table 9: Wyckoff bond: 48c@8b

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

Table 10: Wyckoff bond: 96d@8b

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

Table 11: Wyckoff bond: 96e@8b

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

Table 12: Wyckoff bond: 192f@8b

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

continued ...

Table 12

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

* Wyckoff site: 16c, site symmetry: $\cdot -3m$

Table 13: Wyckoff bond: 16a@16c

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

Table 14: Wyckoff bond: 48b@16c

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

Table 15: Wyckoff bond: 48c@16c

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

Table 16: Wyckoff bond: 96d@16c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -25]$
2	$[-X, -Y, Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[2, -26]$
3	$[-X, Y, -Z]$	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	$[3, -27]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	$[4, -28]$
5	$[Z, X, Y]$	$[0, 0, 0]$	$[5, -29]$
6	$[Z, -X, -Y]$	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	$[6, -30]$
7	$[-Z, -X, Y]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[7, -31]$
8	$[-Z, X, -Y]$	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	$[8, -32]$
9	$[Y, Z, X]$	$[0, 0, 0]$	$[9, -33]$

continued ...

Table 16

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

* Wyckoff site: 16d, site symmetry: $\bar{3}m$

Table 17: Wyckoff bond: 16a@16d

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

Table 18: Wyckoff bond: 48b@16d

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

Table 19: Wyckoff bond: 48c@16d

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

Table 20: Wyckoff bond: 96d@16d

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

* Wyckoff site: 32e, site symmetry: .3m

Table 21: Wyckoff bond: 32a@32e

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

Table 22: Wyckoff bond: 96b@32e

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

Table 23: Wyckoff bond: 96c@32e

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, x]$	$[1, -38]$

continued ...

Table 23

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

Table 24: Wyckoff bond: 192d@32e

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

continued ...

Table 24

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

* Wyckoff site: 48f, site symmetry: 2.mm

Table 25: Wyckoff bond: 48a@48f

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

continued ...

Table 25

No.	vector	center	mapping
9	$[0, X, -X]$	$[x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}]$	$[17, -20, 26, -27]$
10	$[0, X, X]$	$[\frac{1}{2} - x, \frac{7}{8}, \frac{3}{8}]$	$[18, -19, -25, 28]$
11	$[X, X, 0]$	$[\frac{7}{8}, \frac{3}{8}, \frac{1}{2} - x]$	$[21, -24, -33, 36]$
12	$[X, -X, 0]$	$[\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}]$	$[22, -23, 34, -35]$

Table 26: Wyckoff bond: 48b@48f

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

Table 27: Wyckoff bond: 96c@48f

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

continued ...

Table 27

No.	vector	center	mapping
19	$[-Y, -X, -X]$	$[\frac{1}{2} - x, \frac{7}{8}, \frac{3}{8}]$	[19, 25]
20	$[Y, -X, X]$	$[x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}]$	[20, 27]
21	$[X, X, -Y]$	$[\frac{7}{8}, \frac{3}{8}, \frac{1}{2} - x]$	[21, 36]
22	$[X, -X, Y]$	$[\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}]$	[22, 34]
23	$[-X, X, Y]$	$[\frac{3}{8}, \frac{3}{8}, x + \frac{3}{4}]$	[23, 35]
24	$[-X, -X, -Y]$	$[\frac{7}{8}, \frac{3}{8}, \frac{1}{2} - x]$	[24, 33]

Table 28: Wyckoff bond: 96d@48f

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

Table 29: Wyckoff bond: 192e@48f

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

continued ...

Table 29

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

* Wyckoff site: 96g, site symmetry: $\dots m$

Table 30: Wyckoff bond: 96a@96g

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

Table 31: Wyckoff bond: 96b@96g

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

continued ...

Table 31

No.	vector	center	mapping
16	$[X, X, 0]$	$[\frac{1}{2} - x, x + \frac{3}{4}, z + \frac{1}{4}]$	[16, -28]
17	$[X, 0, X]$	$[x + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{2} - x]$	[17, -36]
18	$[-X, 0, -X]$	$[\frac{1}{2} - x, z + \frac{3}{4}, x + \frac{1}{4}]$	[18, -35]
19	$[-X, 0, X]$	$[-x, -z, -x]$	[19, -33]
20	$[X, 0, -X]$	$[x + \frac{1}{4}, \frac{1}{2} - z, x + \frac{3}{4}]$	[20, -34]
21	$[0, -X, -X]$	$[z + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - x]$	[21, -31]
22	$[0, X, X]$	$[z + \frac{1}{4}, \frac{1}{2} - x, x + \frac{3}{4}]$	[22, -32]
23	$[0, -X, X]$	$[\frac{1}{2} - z, x + \frac{3}{4}, x + \frac{1}{4}]$	[23, -30]
24	$[0, X, -X]$	$[-z, -x, -x]$	[24, -29]

Table 32: Wyckoff bond: 192c@96g

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

continued ...

Table 32

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

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

Table 33: Wyckoff bond: 96a@96h

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

continued ...

Table 33

No.	vector	center	mapping
23	$[-X, X, Y]$	$[\frac{1}{2} - y, \frac{1}{4} - y, \frac{3}{4}]$	[35, -47]
24	$[X, X, -Y]$	$[y + \frac{1}{4}, \frac{3}{4} - y, \frac{1}{2}]$	[36, -45]

Table 34: Wyckoff bond: 96b@96h

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

Table 35: Wyckoff bond: 192c@96h

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

continued ...

Table 35

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

* Wyckoff site: 192i, site symmetry: 1

Table 36: Wyckoff bond: 192a@192i

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

continued ...

Table 36

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