SG No. 228 O_{h}^{8} $Fd\bar{3}c$ [cubic]

* plus set: $+[0,\,0,\,0]$, $+\left[0,\,\frac{1}{2},\,\frac{1}{2}\right]$, $+\left[\frac{1}{2},\,0,\,\frac{1}{2}\right]$, $+\left[\frac{1}{2},\,\frac{1}{2},\,0\right]$
* Wyckoff site: `16a`, site symmetry: `23.`

Table 1: Wyckoff bond: `48a@16a`

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

Table 2: Wyckoff bond: `64b@16a`

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

Table 3: Wyckoff bond: `96c@16a`

No.	vector	center	mapping
1	$[X,\,Y,\,0]$	$\left[\frac{1}{8},\,\frac{1}{8},\,\frac{1}{8}\right]$	`[1,-2]`

continued ...

Table 3

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

Table 4: Wyckoff bond: `192d@16a`

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

continued ...

Table 4

No.	vector	center	mapping
18	$[-X, Z, Y]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[18]
19	$[-X, -Z, -Y]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[19]
20	$[X, -Z, Y]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[20]
21	$[Z, Y, -X]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[21]
22	$[Z, -Y, X]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[22]
23	$[-Z, Y, X]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[23]
24	$[-Z, -Y, -X]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[24]
25	$[-X, -Y, -Z]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[25]
26	$[X, Y, -Z]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[26]
27	$[X, -Y, Z]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[27]
28	$[-X, Y, Z]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[28]
29	$[-Z, -X, -Y]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[29]
30	$[-Z, X, Y]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[30]
31	$[Z, X, -Y]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[31]
32	$[Z, -X, Y]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[32]
33	$[-Y, -Z, -X]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[33]
34	$[Y, -Z, X]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[34]
35	$[-Y, Z, X]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[35]
36	$[Y, Z, -X]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[36]
37	$[-Y, -X, Z]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[37]
38	$[Y, X, Z]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[38]
39	$[-Y, X, -Z]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[39]
40	$[Y, -X, -Z]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[40]
41	$[-X, -Z, Y]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[41]
42	$[X, -Z, -Y]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[42]
43	$[X, Z, Y]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[43]
44	$[-X, Z, -Y]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[44]
45	$[-Z, -Y, X]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[45]
46	$[-Z, Y, -X]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[46]
47	$[Z, -Y, -X]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[47]
48	$[Z, Y, X]$	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[48]

* Wyckoff site: 32b, site symmetry: .32

Table 5: Wyckoff bond: 32a@32b

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

Table 6: Wyckoff bond: `96b@32b`

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

Table 7: Wyckoff bond: `96c@32b`

No.	vector	center	mapping
1	$[X, -X, 0]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,14]`
2	$[-X, X, 0]$	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	`[2,13]`
3	$[-X, -X, 0]$	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	`[3,15]`
4	$[X, X, 0]$	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	`[4,16]`
5	$[0, X, -X]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[5,24]`
6	$[0, -X, X]$	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	`[6,23]`
7	$[0, -X, -X]$	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	`[7,21]`
8	$[0, X, X]$	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	`[8,22]`
9	$[-X, 0, X]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[9,19]`
10	$[X, 0, -X]$	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	`[10,20]`
11	$[-X, 0, -X]$	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	`[11,18]`
12	$[X, 0, X]$	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	`[12,17]`
13	$[-X, X, 0]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[25,38]`
14	$[X, -X, 0]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[26,37]`

continued ...

Table 7

No.	vector	center	mapping
15	$[X, X, 0]$	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[27,39]
16	$[-X, -X, 0]$	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[28,40]
17	$[0, -X, X]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[29,48]
18	$[0, X, -X]$	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[30,47]
19	$[0, X, X]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[31,45]
20	$[0, -X, -X]$	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[32,46]
21	$[X, 0, -X]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[33,43]
22	$[-X, 0, X]$	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[34,44]
23	$[X, 0, X]$	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[35,42]
24	$[-X, 0, -X]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[36,41]

Table 8: Wyckoff bond: 192d@32b

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

continued ...

Table 8

No.	vector	center	mapping
31	$[Z, X, -Y]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[31]`
32	$[Z, -X, Y]$	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	`[32]`
33	$[-Y, -Z, -X]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[33]`
34	$[Y, -Z, X]$	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	`[34]`
35	$[-Y, Z, X]$	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[35]`
36	$[Y, Z, -X]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[36]`
37	$[-Y, -X, Z]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[37]`
38	$[Y, X, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[38]`
39	$[-Y, X, -Z]$	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	`[39]`
40	$[Y, -X, -Z]$	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[40]`
41	$[-X, -Z, Y]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[41]`
42	$[X, -Z, -Y]$	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[42]`
43	$[X, Z, Y]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[43]`
44	$[-X, Z, -Y]$	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	`[44]`
45	$[-Z, -Y, X]$	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[45]`
46	$[-Z, Y, -X]$	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	`[46]`
47	$[Z, -Y, -X]$	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[47]`
48	$[Z, Y, X]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[48]`

* Wyckoff site: `32c`, site symmetry: `.-3.`

Table 9: Wyckoff bond: `32a@32c`

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

Table 10: Wyckoff bond: `96b@32c`

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

continued ...

Table 10

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

* Wyckoff site: `48d`, site symmetry: `-4..`

Table 11: Wyckoff bond: `48a@48d`

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

Table 12: Wyckoff bond: `96b@48d`

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

continued ...

Table 12

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

Table 13: Wyckoff bond: `192c@48d`

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

continued ...

Table 13

No.	vector	center	mapping
19	$[-X, -Z, -Y]$	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[19]
20	$[X, -Z, Y]$	$\left[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[20]
21	$[Z, Y, -X]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[21]
22	$[Z, -Y, X]$	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[22]
23	$[-Z, Y, X]$	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[23]
24	$[-Z, -Y, -X]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[24]
25	$[-X, -Y, -Z]$	$\left[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[25]
26	$[X, Y, -Z]$	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[26]
27	$[X, -Y, Z]$	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[27]
28	$[-X, Y, Z]$	$\left[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[28]
29	$[-Z, -X, -Y]$	$\left[\frac{7}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[29]
30	$[-Z, X, Y]$	$\left[\frac{3}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[30]
31	$[Z, X, -Y]$	$\left[\frac{3}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[31]
32	$[Z, -X, Y]$	$\left[\frac{7}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[32]
33	$[-Y, -Z, -X]$	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[33]
34	$[Y, -Z, X]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[34]
35	$[-Y, Z, X]$	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[35]
36	$[Y, Z, -X]$	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[36]
37	$[-Y, -X, Z]$	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[37]
38	$[Y, X, Z]$	$\left[\frac{5}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[38]
39	$[-Y, X, -Z]$	$\left[\frac{5}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[39]
40	$[Y, -X, -Z]$	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[40]
41	$[-X, -Z, Y]$	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[41]
42	$[X, -Z, -Y]$	$\left[\frac{3}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[42]
43	$[X, Z, Y]$	$\left[\frac{3}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[43]
44	$[-X, Z, -Y]$	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[44]
45	$[-Z, -Y, X]$	$\left[\frac{5}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[45]
46	$[-Z, Y, -X]$	$\left[\frac{1}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[46]
47	$[Z, -Y, -X]$	$\left[\frac{1}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[47]
48	$[Z, Y, X]$	$\left[\frac{5}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[48]

* Wyckoff site: 64e, site symmetry: .3.

Table 14: Wyckoff bond: 64a@64e

No.	vector	center	mapping
1	$[X, X, X]$	$[x, x, x]$	[1,5,9]
2	$[-X, -X, X]$	$\left[\frac{1}{4} - x, \frac{3}{4} - x, x + \frac{1}{2}\right]$	[2,7,12]
3	$[-X, X, -X]$	$\left[\frac{3}{4} - x, x + \frac{1}{2}, \frac{1}{4} - x\right]$	[3,8,10]
4	$[X, -X, -X]$	$\left[x + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - x\right]$	[4,6,11]
5	$[X, X, -X]$	$\left[x + \frac{3}{4}, x + \frac{1}{4}, -x\right]$	[13,17,21]
6	$[-X, -X, -X]$	$\left[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[14,19,24]
7	$[X, -X, X]$	$\left[x + \frac{1}{4}, -x, x + \frac{3}{4}\right]$	[15,20,22]
8	$[-X, X, X]$	$\left[-x, x + \frac{3}{4}, x + \frac{1}{4}\right]$	[16,18,23]
9	$[-X, -X, -X]$	$[-x, -x, -x]$	[25,29,33]

continued ...

Table 14

No.	vector	center	mapping
10	$[X, X, -X]$	$\left[x+\frac{3}{4}, x+\frac{1}{4}, \frac{1}{2}-x\right]$	[26,31,36]
11	$[X, -X, X]$	$\left[x+\frac{1}{4}, \frac{1}{2}-x, x+\frac{3}{4}\right]$	[27,32,34]
12	$[-X, X, X]$	$\left[\frac{1}{2}-x, x+\frac{3}{4}, x+\frac{1}{4}\right]$	[28,30,35]
13	$[-X, -X, X]$	$\left[\frac{1}{4}-x, \frac{3}{4}-x, x\right]$	[37,41,45]
14	$[X, X, X]$	$\left[x+\frac{1}{2}, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[38,43,48]
15	$[-X, X, -X]$	$\left[\frac{3}{4}-x, x, \frac{1}{4}-x\right]$	[39,44,46]
16	$[X, -X, -X]$	$\left[x, \frac{1}{4}-x, \frac{3}{4}-x\right]$	[40,42,47]

Table 15: Wyckoff bond: 192b@64e

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

continued ...

Table 15

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

* Wyckoff site: `96f`, site symmetry: `2..`

Table 16: Wyckoff bond: `96a@96f`

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

Table 17: Wyckoff bond: `96b@96f`

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

Table 18: Wyckoff bond: `192c@96f`

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

continued ...

Table 18

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

* Wyckoff site: 96g, site symmetry: ..2

Table 19: Wyckoff bond: 96a@96g

No.	vector	center	mapping
1	$[Y, X, X]$	$\left[\frac{1}{4}, y, -y\right]$	[1,-19]
2	$[-Y, -X, X]$	$\left[0, \frac{3}{4}-y, \frac{1}{2}-y\right]$	[2,-17]
3	$[-Y, X, -X]$	$\left[\frac{1}{2}, y+\frac{1}{2}, y+\frac{1}{4}\right]$	[3,-20]
4	$[Y, -X, -X]$	$\left[\frac{3}{4}, \frac{1}{4}-y, y+\frac{3}{4}\right]$	[4,-18]
5	$[X, Y, X]$	$\left[-y, \frac{1}{4}, y\right]$	[5,-14]

continued ...

Table 19

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

Table 20: Wyckoff bond: 96b@96g

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

continued ...

Table 20

No.	vector	center	mapping
22	$[X, X, 0]$	$\left[y+\frac{1}{4}, y+\frac{1}{2}, 0\right]$	[34,46]
23	$[-X, -X, 0]$	$\left[\frac{1}{2}-y, \frac{3}{4}-y, \frac{1}{2}\right]$	[35,47]
24	$[X, -X, 0]$	$\left[y+\frac{3}{4}, \frac{1}{4}-y, \frac{1}{4}\right]$	[36,45]

Table 21: Wyckoff bond: 192c@96g

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

continued ...

Table 21

No.	vector	center	mapping
38	$[Y,\ X,\ Z]$	$\left[y,\ \frac{3}{4},\ -y\right]$	[38]
39	$[-Y,\ X,\ -Z]$	$\left[\frac{1}{4}-y,\ \frac{1}{4},\ y+\frac{3}{4}\right]$	[39]
40	$[Y,\ -X,\ -Z]$	$\left[y+\frac{1}{2},\ 0,\ y+\frac{1}{4}\right]$	[40]
41	$[-X,\ -Z,\ Y]$	$\left[0,\ y+\frac{1}{4},\ y+\frac{1}{2}\right]$	[41]
42	$[X,\ -Z,\ -Y]$	$\left[\frac{1}{4},\ y+\frac{3}{4},\ \frac{1}{4}-y\right]$	[42]
43	$[X,\ Z,\ Y]$	$\left[\frac{3}{4},\ -y,\ y\right]$	[43]
44	$[-X,\ Z,\ -Y]$	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[44]
45	$[-Z,\ -Y,\ X]$	$\left[y+\frac{3}{4},\ \frac{1}{4}-y,\ \frac{1}{4}\right]$	[45]
46	$[-Z,\ Y,\ -X]$	$\left[y+\frac{1}{4},\ y+\frac{1}{2},\ 0\right]$	[46]
47	$[Z,\ -Y,\ -X]$	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{1}{2}\right]$	[47]
48	$[Z,\ Y,\ X]$	$\left[-y,\ y,\ \frac{3}{4}\right]$	[48]

* Wyckoff site: 192h, site symmetry: 1

Table 22: Wyckoff bond: 192a@192h

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

continued ...

Table 22

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