SG No. 230 O_{h}^{10} $Ia\bar{3}d$ [cubic]

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

* Wyckoff site: `16a`, site symmetry: `.-3.`

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

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

Table 2: Wyckoff bond: `48b@16a`

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

* Wyckoff site: `16b`, site symmetry: `.32`

Table 3: Wyckoff bond: `16a@16b`

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

Table 4: Wyckoff bond: `48b@16b`

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

Table 5: Wyckoff bond: `48c@16b`

No.	vector	center	mapping
1	$[X, -X, 0]$	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[1,14]

continued ...

Table 5

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

Table 6: Wyckoff bond: `96d@16b`

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

Table 6

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

* Wyckoff site: 24c, site symmetry: 2.22

Table 7: Wyckoff bond: 24a@24c

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

Table 7

No.	vector	center	mapping
9	$[-X, 0, -X]$	$\left[\frac{3}{4}, \frac{7}{8}, 0\right]$	[29,-32,-38,39]
10	$[-X, 0, X]$	$\left[\frac{1}{4}, \frac{5}{8}, 0\right]$	[30,-31,37,-40]
11	$[-X, -X, 0]$	$\left[0, \frac{3}{4}, \frac{7}{8}\right]$	[33,-36,45,-48]
12	$[X, -X, 0]$	$\left[0, \frac{1}{4}, \frac{5}{8}\right]$	[34,-35,-46,47]

Table 8: Wyckoff bond: `24b@24c`

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

Table 9: Wyckoff bond: `24c@24c`

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

Table 10: Wyckoff bond: `48d@24c`

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

Table 11: Wyckoff bond: `48e@24c`

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

continued …

Table 11

No.	vector	center	mapping
16	$[-Y, X, -X]$	$\left[\frac{7}{8}, 0, \frac{3}{4}\right]$	[28,-43]
17	$[X, -Y, -X]$	$\left[\frac{3}{4}, \frac{7}{8}, 0\right]$	[29,-39]
18	$[X, Y, X]$	$\left[\frac{1}{4}, \frac{5}{8}, 0\right]$	[30,-37]
19	$[-X, Y, -X]$	$\left[\frac{1}{4}, \frac{5}{8}, 0\right]$	[31,-40]
20	$[-X, -Y, X]$	$\left[\frac{3}{4}, \frac{7}{8}, 0\right]$	[32,-38]
21	$[-X, X, -Y]$	$\left[0, \frac{3}{4}, \frac{7}{8}\right]$	[33,-45]
22	$[X, X, Y]$	$\left[0, \frac{1}{4}, \frac{5}{8}\right]$	[34,-47]
23	$[-X, -X, Y]$	$\left[0, \frac{1}{4}, \frac{5}{8}\right]$	[35,-46]
24	$[X, -X, -Y]$	$\left[0, \frac{3}{4}, \frac{7}{8}\right]$	[36,-48]

Table 12: Wyckoff bond: `48f@24c`

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

Table 13: Wyckoff bond: `96g@24c`

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

continued ...

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Table 13

No.	vector	center	mapping
47	$[Z, -Y, -X]$	$\left[0, \frac{1}{4}, \frac{5}{8}\right]$	[47]
48	$[Z, Y, X]$	$\left[0, \frac{3}{4}, \frac{7}{8}\right]$	[48]

* Wyckoff site: `24d`, site symmetry: `-4..`

Table 14: Wyckoff bond: `24a@24d`

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

Table 15: Wyckoff bond: `48b@24d`

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

continued ...

Table 15

No.	vector	center	mapping
19	$[-X, 0, Y]$	$\left[\frac{1}{4}, \frac{3}{8}, 0\right]$	[37,-40]
20	$[X, 0, Y]$	$\left[\frac{3}{4}, \frac{1}{8}, 0\right]$	[38,-39]
21	$[0, -Y, X]$	$\left[\frac{3}{8}, 0, \frac{1}{4}\right]$	[41,-44]
22	$[0, -Y, -X]$	$\left[\frac{1}{8}, 0, \frac{3}{4}\right]$	[42,-43]
23	$[-Y, -X, 0]$	$\left[0, \frac{3}{4}, \frac{1}{8}\right]$	[45,-48]
24	$[-Y, X, 0]$	$\left[0, \frac{1}{4}, \frac{3}{8}\right]$	[46,-47]

Table 16: Wyckoff bond: `96c@24d`

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

continued ...

Table 16

No.	vector	center	mapping
35	$[-Y, Z, X]$	$\left[0, \frac{1}{4}, \frac{7}{8}\right]$	[35]
36	$[Y, Z, -X]$	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{8}\right]$	[36]
37	$[-Y, -X, Z]$	$\left[\frac{1}{4}, \frac{3}{8}, 0\right]$	[37]
38	$[Y, X, Z]$	$\left[\frac{3}{4}, \frac{1}{8}, 0\right]$	[38]
39	$[-Y, X, -Z]$	$\left[\frac{3}{4}, \frac{1}{8}, 0\right]$	[39]
40	$[Y, -X, -Z]$	$\left[\frac{1}{4}, \frac{3}{8}, 0\right]$	[40]
41	$[-X, -Z, Y]$	$\left[\frac{3}{8}, 0, \frac{1}{4}\right]$	[41]
42	$[X, -Z, -Y]$	$\left[\frac{1}{8}, 0, \frac{3}{4}\right]$	[42]
43	$[X, Z, Y]$	$\left[\frac{1}{8}, 0, \frac{3}{4}\right]$	[43]
44	$[-X, Z, -Y]$	$\left[\frac{3}{8}, 0, \frac{1}{4}\right]$	[44]
45	$[-Z, -Y, X]$	$\left[0, \frac{3}{4}, \frac{1}{8}\right]$	[45]
46	$[-Z, Y, -X]$	$\left[0, \frac{1}{4}, \frac{3}{8}\right]$	[46]
47	$[Z, -Y, -X]$	$\left[0, \frac{1}{4}, \frac{3}{8}\right]$	[47]
48	$[Z, Y, X]$	$\left[0, \frac{3}{4}, \frac{1}{8}\right]$	[48]

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

Table 17: Wyckoff bond: 32a@32e

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

Table 18: Wyckoff bond: 96b@32e

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

continued ...

Table 18

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

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

Table 19: Wyckoff bond: `48a@48f`

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

Table 20: Wyckoff bond: `48b@48f`

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

continued ...

Table 20

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

Table 21: Wyckoff bond: `96c@48f`

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

continued ...

Table 21

No.	vector	center	mapping
29	$[-Z, -X, -Y]$	$\left[\frac{3}{4}, -x, 0\right]$	[29]
30	$[-Z, X, Y]$	$\left[\frac{1}{4}, x+\frac{1}{2}, 0\right]$	[30]
31	$[Z, X, -Y]$	$\left[\frac{1}{4}, x+\frac{1}{2}, 0\right]$	[31]
32	$[Z, -X, Y]$	$\left[\frac{3}{4}, -x, 0\right]$	[32]
33	$[-Y, -Z, -X]$	$\left[0, \frac{3}{4}, -x\right]$	[33]
34	$[Y, -Z, X]$	$\left[0, \frac{1}{4}, x+\frac{1}{2}\right]$	[34]
35	$[-Y, Z, X]$	$\left[0, \frac{1}{4}, x+\frac{1}{2}\right]$	[35]
36	$[Y, Z, -X]$	$\left[0, \frac{3}{4}, -x\right]$	[36]
37	$[-Y, -X, Z]$	$\left[\frac{1}{4}, \frac{3}{4}-x, 0\right]$	[37]
38	$[Y, X, Z]$	$\left[\frac{1}{4}, x+\frac{1}{4}, \frac{1}{2}\right]$	[38]
39	$[-Y, X, -Z]$	$\left[\frac{1}{4}, x+\frac{1}{4}, \frac{1}{2}\right]$	[39]
40	$[Y, -X, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}-x, 0\right]$	[40]
41	$[-X, -Z, Y]$	$\left[\frac{1}{4}-x, \frac{1}{2}, \frac{3}{4}\right]$	[41]
42	$[X, -Z, -Y]$	$\left[x+\frac{3}{4}, 0, \frac{3}{4}\right]$	[42]
43	$[X, Z, Y]$	$\left[x+\frac{3}{4}, 0, \frac{3}{4}\right]$	[43]
44	$[-X, Z, -Y]$	$\left[\frac{1}{4}-x, \frac{1}{2}, \frac{3}{4}\right]$	[44]
45	$[-Z, -Y, X]$	$\left[0, \frac{3}{4}, x+\frac{3}{4}\right]$	[45]
46	$[-Z, Y, -X]$	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}-x\right]$	[46]
47	$[Z, -Y, -X]$	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}-x\right]$	[47]
48	$[Z, Y, X]$	$\left[0, \frac{3}{4}, x+\frac{3}{4}\right]$	[48]

* Wyckoff site: 48g, site symmetry: ..2

Table 22: Wyckoff bond: 48a@48g

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

Table 22

No.	vector	center	mapping
20	$[X, -Y, X]$	$\left[\frac{1}{4} - y, \frac{3}{8}, y + \frac{1}{2}\right]$	[32,-39]
21	$[-X, -X, -Y]$	$\left[-y, y + \frac{3}{4}, \frac{7}{8}\right]$	[33,-48]
22	$[X, -X, Y]$	$\left[y, y + \frac{1}{4}, \frac{5}{8}\right]$	[34,-46]
23	$[-X, X, Y]$	$\left[\frac{1}{2} - y, \frac{3}{4} - y, \frac{1}{8}\right]$	[35,-47]
24	$[X, X, -Y]$	$\left[y + \frac{1}{2}, \frac{1}{4} - y, \frac{3}{8}\right]$	[36,-45]

Table 23: Wyckoff bond: `48b@48g`

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

Table 24: Wyckoff bond: `96c@48g`

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

continued ...

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Table 24

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

* Wyckoff site: 96h, site symmetry: 1

Table 25: Wyckoff bond: `96a@96h`

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

continued ...

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Table 25

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

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