

SG No. 203 $T_h^4 Fd\bar{3}$ [cubic]

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

* Wyckoff site: **8a**, site symmetry: **23**.

Table 1: Wyckoff bond: **24a@8a**

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

Table 2: Wyckoff bond: **32b@8a**

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

Table 3: Wyckoff bond: **48c@8a**

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

Table 4: Wyckoff bond: 96d@8a

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

* Wyckoff site: 8b, site symmetry: 23.

Table 5: Wyckoff bond: 24a@8b

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

Table 6: Wyckoff bond: 32b@8b

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

continued ...

Table 6

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

Table 7: Wyckoff bond: 48c@8b

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

Table 8: Wyckoff bond: 96d@8b

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

continued ...

Table 8

No.	vector	center	mapping
17	$[-Z, -X, -Y]$	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[17]
18	$[-Z, X, Y]$	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[18]
19	$[Z, X, -Y]$	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[19]
20	$[Z, -X, Y]$	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[20]
21	$[-Y, -Z, -X]$	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[21]
22	$[Y, -Z, X]$	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[22]
23	$[-Y, Z, X]$	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[23]
24	$[Y, Z, -X]$	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[24]

* Wyckoff site: 16c, site symmetry: $\bar{3}$.

Table 9: Wyckoff bond: 16a@16c

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

Table 10: Wyckoff bond: 48b@16c

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

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

Table 11: Wyckoff bond: 16a@16d

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

Table 12: Wyckoff bond: 48b@16d

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

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

Table 13: Wyckoff bond: 32a@32e

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

Table 14: Wyckoff bond: 96b@32e

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, x]$	$[1]$

continued ...

Table 14

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

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

Table 15: Wyckoff bond: 48a@48f

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

Table 16: Wyckoff bond: 48b@48f

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

Table 17: Wyckoff bond: 96c@48f

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

* Wyckoff site: 96g, site symmetry: 1

Table 18: Wyckoff bond: 96a@96g

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