

SG No. 210 O^4 $F4_132$ [cubic]

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

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

Table 1: Wyckoff bond: 24a@8a

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

Table 2: Wyckoff bond: 32b@8a

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

Table 3: Wyckoff bond: 48c@8a

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

Table 4: Wyckoff bond: 96d@8a

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

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

Table 5: Wyckoff bond: 24a@8b

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

Table 6: Wyckoff bond: 32b@8b

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

continued ...

Table 6

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

Table 7: Wyckoff bond: 48c@8b

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

Table 8: Wyckoff bond: 96d@8b

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

continued ...

Table 8

No.	vector	center	mapping
17	$[X, Z, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[17]
18	$[-X, Z, Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[19]
20	$[X, -Z, Y]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[20]
21	$[Z, Y, -X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[21]
22	$[Z, -Y, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[22]
23	$[-Z, Y, X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[24]

* Wyckoff site: 16c, site symmetry: .32

Table 9: Wyckoff bond: 16a@16c

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

Table 10: Wyckoff bond: 48b@16c

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

Table 11: Wyckoff bond: 48c@16c

No.	vector	center	mapping
1	$[X, -X, 0]$	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[1,14]
2	$[-X, X, 0]$	$[\frac{7}{8}, \frac{3}{8}, \frac{5}{8}]$	[2,13]

continued ...

Table 11

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

Table 12: Wyckoff bond: 96d@16c

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

* Wyckoff site: 16d, site symmetry: .32

Table 13: Wyckoff bond: 16a@16d

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

Table 14: Wyckoff bond: 48b@16d

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

Table 15: Wyckoff bond: 48c@16d

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

Table 16: Wyckoff bond: 96d@16d

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

* 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	$[-X, -X, X]$	$[-x, \frac{1}{2} - x, x + \frac{1}{2}]$	[2,7,12]
3	$[-X, X, -X]$	$[\frac{1}{2} - x, x + \frac{1}{2}, -x]$	[3,8,10]
4	$[X, -X, -X]$	$[x + \frac{1}{2}, -x, \frac{1}{2} - x]$	[4,6,11]
5	$[X, X, -X]$	$[x + \frac{3}{4}, x + \frac{1}{4}, \frac{3}{4} - x]$	[13,17,21]
6	$[-X, -X, -X]$	$[\frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x]$	[14,19,24]
7	$[X, -X, X]$	$[x + \frac{1}{4}, \frac{3}{4} - x, x + \frac{3}{4}]$	[15,20,22]
8	$[-X, X, X]$	$[\frac{3}{4} - x, x + \frac{3}{4}, x + \frac{1}{4}]$	[16,18,23]

Table 18: Wyckoff bond: 96b@32e

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

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

Table 19: Wyckoff bond: 48a@48f

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

Table 20: Wyckoff bond: 48b@48f

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

Table 21: Wyckoff bond: 96c@48f

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

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

Table 22: Wyckoff bond: 48a@48g

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

Table 23: Wyckoff bond: 48b@48g

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

Table 24: Wyckoff bond: 96c@48g

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

continued ...

Table 24

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

* 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	$[-X, -Y, Z]$	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[2]
3	$[-X, Y, -Z]$	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[3]
4	$[X, -Y, -Z]$	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[4]
5	$[Z, X, Y]$	$[z, x, y]$	[5]
6	$[Z, -X, -Y]$	$[z + \frac{1}{2}, -x, \frac{1}{2} - y]$	[6]
7	$[-Z, -X, Y]$	$[-z, \frac{1}{2} - x, y + \frac{1}{2}]$	[7]
8	$[-Z, X, -Y]$	$[\frac{1}{2} - z, x + \frac{1}{2}, -y]$	[8]
9	$[Y, Z, X]$	$[y, z, x]$	[9]
10	$[-Y, Z, -X]$	$[\frac{1}{2} - y, z + \frac{1}{2}, -x]$	[10]
11	$[Y, -Z, -X]$	$[y + \frac{1}{2}, -z, \frac{1}{2} - x]$	[11]
12	$[-Y, -Z, X]$	$[-y, \frac{1}{2} - z, x + \frac{1}{2}]$	[12]
13	$[Y, X, -Z]$	$[y + \frac{3}{4}, x + \frac{1}{4}, \frac{3}{4} - z]$	[13]
14	$[-Y, -X, -Z]$	$[\frac{1}{4} - y, \frac{1}{4} - x, \frac{1}{4} - z]$	[14]
15	$[Y, -X, Z]$	$[y + \frac{1}{4}, \frac{3}{4} - x, z + \frac{3}{4}]$	[15]
16	$[-Y, X, Z]$	$[\frac{3}{4} - y, x + \frac{3}{4}, z + \frac{1}{4}]$	[16]
17	$[X, Z, -Y]$	$[x + \frac{3}{4}, z + \frac{1}{4}, \frac{3}{4} - y]$	[17]
18	$[-X, Z, Y]$	$[\frac{3}{4} - x, z + \frac{3}{4}, y + \frac{1}{4}]$	[18]
19	$[-X, -Z, -Y]$	$[\frac{1}{4} - x, \frac{1}{4} - z, \frac{1}{4} - y]$	[19]
20	$[X, -Z, Y]$	$[x + \frac{1}{4}, \frac{3}{4} - z, y + \frac{3}{4}]$	[20]
21	$[Z, Y, -X]$	$[z + \frac{3}{4}, y + \frac{1}{4}, \frac{3}{4} - x]$	[21]
22	$[Z, -Y, X]$	$[z + \frac{1}{4}, \frac{3}{4} - y, x + \frac{3}{4}]$	[22]
23	$[-Z, Y, X]$	$[\frac{3}{4} - z, y + \frac{3}{4}, x + \frac{1}{4}]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{4} - z, \frac{1}{4} - y, \frac{1}{4} - x]$	[24]

