

SG No. 219 T_d^5 $F\bar{4}3c$ [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	$[X, 0, 0]$	$[0, 0, 0]$	$[1, -2, -3, 4]$
2	$[0, X, 0]$	$[0, 0, 0]$	$[5, -6, -7, 8]$
3	$[0, 0, X]$	$[0, 0, 0]$	$[9, -10, -11, 12]$
4	$[0, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[13, -14, -15, 16]$
5	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[17, -18, -19, 20]$
6	$[0, 0, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[21, -22, -23, 24]$

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	$[X, X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[13, 17, 21]$
6	$[-X, -X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[14, 19, 24]$
7	$[X, -X, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[15, 20, 22]$
8	$[-X, X, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[16, 18, 23]$

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	$[Y, X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[13, -14]$
8	$[Y, -X, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[15, -16]$
9	$[X, 0, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[17, -18]$
10	$[-X, 0, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[19, -20]$
11	$[0, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[21, -22]$
12	$[0, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[23, -24]$

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	$[Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[13]
14	$[-Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[14]
15	$[Y, -X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[15]
16	$[-Y, X, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[16]
17	$[X, Z, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[17]
18	$[-X, Z, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[18]
19	$[-X, -Z, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[19]
20	$[X, -Z, -Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[20]
21	$[Z, Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[21]
22	$[Z, -Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[22]
23	$[-Z, Y, -X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[23]
24	$[-Z, -Y, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[24]

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

Table 5: Wyckoff bond: 24a@8b

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

Table 6: Wyckoff bond: 32b@8b

No.	vector	center	mapping
1	$[X, X, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1, 5, 9]
2	$[-X, -X, X]$	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[2, 7, 12]

continued ...

Table 6

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

Table 7: Wyckoff bond: 48c@8b

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

Table 8: Wyckoff bond: 96d@8b

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

continued ...

Table 8

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

* Wyckoff site: 24c, site symmetry: $-4..$

Table 9: Wyckoff bond: 24a@24c

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

Table 10: Wyckoff bond: 48b@24c

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

Table 11: Wyckoff bond: 96c@24c

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

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

Table 12: Wyckoff bond: 24a@24d

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

Table 13: Wyckoff bond: 48b@24d

No.	vector	center	mapping
1	$[0, X, Y]$	$[\frac{1}{4}, 0, 0]$	[1, -4]
2	$[0, -X, Y]$	$[\frac{3}{4}, 0, 0]$	[2, -3]

continued ...

Table 13

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

Table 14: Wyckoff bond: 96c@24d

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

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

Table 15: Wyckoff bond: 32a@32e

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

Table 16: Wyckoff bond: 96b@32e

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

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

Table 17: Wyckoff bond: **48a@48f**

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

Table 18: Wyckoff bond: **48b@48f**

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

Table 19: Wyckoff bond: **96c@48f**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, 0, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, 0, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[x, 0, 0]$	$[4]$
5	$[Z, X, Y]$	$[0, x, 0]$	$[5]$
6	$[Z, -X, -Y]$	$[0, -x, 0]$	$[6]$
7	$[-Z, -X, Y]$	$[0, -x, 0]$	$[7]$
8	$[-Z, X, -Y]$	$[0, x, 0]$	$[8]$
9	$[Y, Z, X]$	$[0, 0, x]$	$[9]$

continued ...

Table 19

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

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

Table 20: Wyckoff bond: **48a@48g**

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

Table 21: Wyckoff bond: **48b@48g**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, \frac{1}{4}, \frac{1}{4}]$	[1,4]
2	$[-X, 0, 0]$	$[-x, \frac{3}{4}, \frac{1}{4}]$	[2,3]
3	$[0, X, 0]$	$[\frac{1}{4}, x, \frac{1}{4}]$	[5,8]
4	$[0, -X, 0]$	$[\frac{1}{4}, -x, \frac{3}{4}]$	[6,7]
5	$[0, 0, X]$	$[\frac{1}{4}, \frac{1}{4}, x]$	[9,12]

continued ...

Table 21

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

Table 22: Wyckoff bond: 96c@48g

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

* Wyckoff site: 96h, site symmetry: 1

Table 23: Wyckoff bond: 96a@96h

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

continued ...

Table 23

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