SG No. 209 O^3 $F432$ [cubic]

Table 1: Wyckoff bond: 12a@4a

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

Table 2: Wyckoff bond: 16b@4a

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

Table 3: Wyckoff bond: 24c@4a

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

Table 4: Wyckoff bond: 48d@4a

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

Table 4

No.	vector	center	mapping
11	$[X, -Y, -X]$	$[0, 0, 0]$	[11,-18]
12	$[-X, -Y, X]$	$[0, 0, 0]$	[12,-17]

Table 5: Wyckoff bond: `48e@4a`

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

Table 6: Wyckoff bond: `96f@4a`

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	$[Y, X, -Z]$	$[0, 0, 0]$	[13]
14	$[-Y, -X, -Z]$	$[0, 0, 0]$	[14]
15	$[Y, -X, Z]$	$[0, 0, 0]$	[15]
16	$[-Y, X, Z]$	$[0, 0, 0]$	[16]
17	$[X, Z, -Y]$	$[0, 0, 0]$	[17]
18	$[-X, Z, Y]$	$[0, 0, 0]$	[18]
19	$[-X, -Z, -Y]$	$[0, 0, 0]$	[19]
20	$[X, -Z, Y]$	$[0, 0, 0]$	[20]

continued …

Table 6

No.	vector	center	mapping
21	$[Z, Y, -X]$	$[0, 0, 0]$	[21]
22	$[Z, -Y, X]$	$[0, 0, 0]$	[22]
23	$[-Z, Y, X]$	$[0, 0, 0]$	[23]
24	$[-Z, -Y, -X]$	$[0, 0, 0]$	[24]

* Wyckoff site: 4b, site symmetry: 432

Table 7: Wyckoff bond: 12a@4b

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

Table 8: Wyckoff bond: 16b@4b

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

Table 9: Wyckoff bond: 24c@4b

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

Table 10: Wyckoff bond: 48d@4b

No.	vector	center	mapping
1	$[X, X, Y]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[1,-14]
2	$[-X, -X, Y]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[2,-13]
3	$[-X, X, -Y]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[3,-15]

continued …

Table 10

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

Table 11: Wyckoff bond: `48e@4b`

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

Table 12: Wyckoff bond: `96f@4b`

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

continued ...

Table 12

No.	vector	center	mapping
14	$[-Y, -X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[14]
15	$[Y, -X, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[15]
16	$[-Y, X, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[16]
17	$[X, Z, -Y]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[17]
18	$[-X, Z, Y]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[18]
19	$[-X, -Z, -Y]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[19]
20	$[X, -Z, Y]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[20]
21	$[Z, Y, -X]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[21]
22	$[Z, -Y, X]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[22]
23	$[-Z, Y, X]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[23]
24	$[-Z, -Y, -X]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[24]

* Wyckoff site: `8c`, site symmetry: `23`.

Table 13: Wyckoff bond: `24a@8c`

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

Table 14: Wyckoff bond: `32b@8c`

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

Table 15: Wyckoff bond: `48c@8c`

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

continued ...

Table 15

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

Table 16: Wyckoff bond: `96d@8c`

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

* Wyckoff site: `24d`, site symmetry: `2.22`

Table 17: Wyckoff bond: `24a@24d`

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

Table 18: Wyckoff bond: `24b@24d`

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

Table 19: Wyckoff bond: `24c@24d`

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

Table 20: Wyckoff bond: `48d@24d`

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

continued ...

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Table 20

No.	vector	center	mapping
10	$[-X, X, -Y]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[10,-22]
11	$[X, -X, -Y]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[11,-23]
12	$[-X, -X, Y]$	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[12,-21]

Table 21: Wyckoff bond: `48e@24d`

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

Table 22: Wyckoff bond: `48f@24d`

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

Table 23: Wyckoff bond: `96g@24d`

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	$[Z, Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, 0]$	[21]
22	$[Z, -Y, X]$	$[\frac{3}{4}, \frac{1}{4}, 0]$	[22]
23	$[-Z, Y, X]$	$[\frac{3}{4}, \frac{1}{4}, 0]$	[23]
24	$[-Z, -Y, -X]$	$[\frac{1}{4}, \frac{1}{4}, 0]$	[24]

* Wyckoff site: `24e`, site symmetry: `4..`

Table 24: Wyckoff bond: `24a@24e`

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

Table 25: Wyckoff bond: `48b@24e`

No.	vector	center	mapping
1	$[0, X, Y]$	$[x, 0, 0]$	[1,-4]
2	$[0, -X, Y]$	$[-x, 0, 0]$	[2,-3]

continued ...

Table 25

No.	vector	center	mapping
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	$[X, 0, -Y]$	$[0, x, 0]$	[13,-16]
8	$[-X, 0, -Y]$	$[0, -x, 0]$	[14,-15]
9	$[0, Y, -X]$	$[x, 0, 0]$	[17,-20]
10	$[0, Y, X]$	$[-x, 0, 0]$	[18,-19]
11	$[Y, X, 0]$	$[0, 0, -x]$	[21,-24]
12	$[Y, -X, 0]$	$[0, 0, x]$	[22,-23]

Table 26: Wyckoff bond: `96c@24e`

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]
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	$[Y, X, -Z]$	$[0, x, 0]$	[13]
14	$[-Y, -X, -Z]$	$[0, -x, 0]$	[14]
15	$[Y, -X, Z]$	$[0, -x, 0]$	[15]
16	$[-Y, X, Z]$	$[0, x, 0]$	[16]
17	$[X, Z, -Y]$	$[x, 0, 0]$	[17]
18	$[-X, Z, Y]$	$[-x, 0, 0]$	[18]
19	$[-X, -Z, -Y]$	$[-x, 0, 0]$	[19]
20	$[X, -Z, Y]$	$[x, 0, 0]$	[20]
21	$[Z, Y, -X]$	$[0, 0, -x]$	[21]
22	$[Z, -Y, X]$	$[0, 0, x]$	[22]
23	$[-Z, Y, X]$	$[0, 0, x]$	[23]
24	$[-Z, -Y, -X]$	$[0, 0, -x]$	[24]

* Wyckoff site: `32f`, site symmetry: `.3.`

Table 27: Wyckoff bond: `32a@32f`

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	$[X, X, -X]$	$[x, x, -x]$	`[13,17,21]`
6	$[-X, -X, -X]$	$[-x, -x, -x]$	`[14,19,24]`
7	$[X, -X, X]$	$[x, -x, x]$	`[15,20,22]`
8	$[-X, X, X]$	$[-x, x, x]$	`[16,18,23]`

Table 28: Wyckoff bond: `96b@32f`

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	$[Y, X, -Z]$	$[x, x, -x]$	`[13]`
14	$[-Y, -X, -Z]$	$[-x, -x, -x]$	`[14]`
15	$[Y, -X, Z]$	$[x, -x, x]$	`[15]`
16	$[-Y, X, Z]$	$[-x, x, x]$	`[16]`
17	$[X, Z, -Y]$	$[x, x, -x]$	`[17]`
18	$[-X, Z, Y]$	$[-x, x, x]$	`[18]`
19	$[-X, -Z, -Y]$	$[-x, -x, -x]$	`[19]`
20	$[X, -Z, Y]$	$[x, -x, x]$	`[20]`
21	$[Z, Y, -X]$	$[x, x, -x]$	`[21]`
22	$[Z, -Y, X]$	$[x, -x, x]$	`[22]`
23	$[-Z, Y, X]$	$[-x, x, x]$	`[23]`
24	$[-Z, -Y, -X]$	$[-x, -x, -x]$	`[24]`

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

Table 29: Wyckoff bond: `48a@48g`

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

Table 30: Wyckoff bond: `48b@48g`

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

Table 31: Wyckoff bond: `96c@48g`

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

continued ...

Table 31

No.	vector	center	mapping
10	$[-Y, Z, -X]$	$[-y, y, 0]$	[10]
11	$[Y, -Z, -X]$	$[y, -y, 0]$	[11]
12	$[-Y, -Z, X]$	$[-y, -y, 0]$	[12]
13	$[Y, X, -Z]$	$[y, 0, -y]$	[13]
14	$[-Y, -X, -Z]$	$[-y, 0, -y]$	[14]
15	$[Y, -X, Z]$	$[y, 0, y]$	[15]
16	$[-Y, X, Z]$	$[-y, 0, y]$	[16]
17	$[X, Z, -Y]$	$[0, y, -y]$	[17]
18	$[-X, Z, Y]$	$[0, y, y]$	[18]
19	$[-X, -Z, -Y]$	$[0, -y, -y]$	[19]
20	$[X, -Z, Y]$	$[0, -y, y]$	[20]
21	$[Z, Y, -X]$	$[y, y, 0]$	[21]
22	$[Z, -Y, X]$	$[y, -y, 0]$	[22]
23	$[-Z, Y, X]$	$[-y, y, 0]$	[23]
24	$[-Z, -Y, -X]$	$[-y, -y, 0]$	[24]

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

Table 32: Wyckoff bond: `48a@48h`

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

Table 33: Wyckoff bond: `48b@48h`

No.	vector	center	mapping
1	$[0, X, X]$	$\left[\frac{1}{2}, y, y\right]$	[1,18]
2	$[0, -X, X]$	$\left[\frac{1}{2}, -y, y\right]$	[2,20]
3	$[0, X, -X]$	$\left[\frac{1}{2}, y, -y\right]$	[3,17]
4	$[0, -X, -X]$	$\left[\frac{1}{2}, -y, -y\right]$	[4,19]
5	$[X, 0, X]$	$\left[y, \frac{1}{2}, y\right]$	[5,15]

continued ...

Table 33

No.	vector	center	mapping
6	$[X, 0, -X]$	$\left[y, \frac{1}{2}, -y\right]$	[6,13]
7	$[-X, 0, X]$	$\left[-y, \frac{1}{2}, y\right]$	[7,16]
8	$[-X, 0, -X]$	$\left[-y, \frac{1}{2}, -y\right]$	[8,14]
9	$[X, X, 0]$	$\left[y, y, \frac{1}{2}\right]$	[9,21]
10	$[-X, X, 0]$	$\left[-y, y, \frac{1}{2}\right]$	[10,23]
11	$[X, -X, 0]$	$\left[y, -y, \frac{1}{2}\right]$	[11,22]
12	$[-X, -X, 0]$	$\left[-y, -y, \frac{1}{2}\right]$	[12,24]

Table 34: Wyckoff bond: `96c@48h`

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

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

Table 35: Wyckoff bond: `48a@48i`

No.	vector	center	mapping
1	$[0, X, Y]$	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	[1,-4]

continued ...

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Table 35

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

Table 36: Wyckoff bond: `48b@48i`

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

Table 37: Wyckoff bond: `96c@48i`

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

Table 37

No.	vector	center	mapping
12	$[-Y, -Z, X]$	$\left[\frac{1}{4}, \frac{1}{4}, x\right]$	[12]
13	$[Y, X, -Z]$	$\left[\frac{1}{4}, x, \frac{3}{4}\right]$	[13]
14	$[-Y, -X, -Z]$	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[14]
15	$[Y, -X, Z]$	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[15]
16	$[-Y, X, Z]$	$\left[\frac{1}{4}, x, \frac{3}{4}\right]$	[16]
17	$[X, Z, -Y]$	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	[17]
18	$[-X, Z, Y]$	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	[18]
19	$[-X, -Z, -Y]$	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	[19]
20	$[X, -Z, Y]$	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	[20]
21	$[Z, Y, -X]$	$\left[\frac{1}{4}, \frac{1}{4}, -x\right]$	[21]
22	$[Z, -Y, X]$	$\left[\frac{1}{4}, \frac{3}{4}, x\right]$	[22]
23	$[-Z, Y, X]$	$\left[\frac{1}{4}, \frac{3}{4}, x\right]$	[23]
24	$[-Z, -Y, -X]$	$\left[\frac{1}{4}, \frac{1}{4}, -x\right]$	[24]

* Wyckoff site: 96j, site symmetry: 1

Table 38: Wyckoff bond: 96a@96j

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
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	$[Y, X, -Z]$	$[y, x, -z]$	[13]
14	$[-Y, -X, -Z]$	$[-y, -x, -z]$	[14]
15	$[Y, -X, Z]$	$[y, -x, z]$	[15]
16	$[-Y, X, Z]$	$[-y, x, z]$	[16]
17	$[X, Z, -Y]$	$[x, z, -y]$	[17]
18	$[-X, Z, Y]$	$[-x, z, y]$	[18]
19	$[-X, -Z, -Y]$	$[-x, -z, -y]$	[19]
20	$[X, -Z, Y]$	$[x, -z, y]$	[20]
21	$[Z, Y, -X]$	$[z, y, -x]$	[21]
22	$[Z, -Y, X]$	$[z, -y, x]$	[22]
23	$[-Z, Y, X]$	$[-z, y, x]$	[23]
24	$[-Z, -Y, -X]$	$[-z, -y, -x]$	[24]