SG No. 214 O^8 $I4_132$ [cubic]

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

* Wyckoff site: `8a`, site symmetry: `.32`

Table 1: Wyckoff bond: `8a@8a`

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]

Table 2: Wyckoff bond: `24b@8a`

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]

Table 3: Wyckoff bond: `24c@8a`

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

Table 4: Wyckoff bond: `48d@8a`

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]
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]

* Wyckoff site: `8b`, site symmetry: `.32`

Table 5: Wyckoff bond: `8a@8b`

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

Table 6: Wyckoff bond: `24b@8b`

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

Table 6

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

Table 7: Wyckoff bond: `24c@8b`

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

Table 8: Wyckoff bond: `48d@8b`

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

continued ...

3

Table 8

No.	vector	center	mapping
15	$[Y, -X, Z]$	$\left[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[15]
16	$[-Y, X, Z]$	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[16]
17	$[X, Z, -Y]$	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[17]
18	$[-X, Z, Y]$	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[18]
19	$[-X, -Z, -Y]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[19]
20	$[X, -Z, Y]$	$\left[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[20]
21	$[Z, Y, -X]$	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[21]
22	$[Z, -Y, X]$	$\left[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[22]
23	$[-Z, Y, X]$	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[23]
24	$[-Z, -Y, -X]$	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[24]

* Wyckoff site: `12c`, site symmetry: `2.22`

Table 9: Wyckoff bond: `12a@12c`

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]

Table 10: Wyckoff bond: `12b@12c`

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]

Table 11: Wyckoff bond: `12c@12c`

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]

continued ...

Table 11

No.	vector	center	mapping
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]

Table 12: Wyckoff bond: `24d@12c`

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]

Table 13: Wyckoff bond: `24e@12c`

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]

Table 14: Wyckoff bond: `24f@12c`

No.	vector	center	mapping
1	$[0, X, Y]$	$\left[\frac{1}{8}, 0, \frac{1}{4}\right]$	[1,-4]

Table 14

No.	vector	center	mapping
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]

Table 15: Wyckoff bond: `48g@12c`

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]

* Wyckoff site: `12d`, site symmetry: `2.22`

Table 16: Wyckoff bond: `12a@12d`

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

Table 17: Wyckoff bond: `12b@12d`

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

Table 18: Wyckoff bond: `12c@12d`

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

Table 19: Wyckoff bond: `24d@12d`

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

continued ...

7

Table 19

No.	vector	center	mapping
10	$[-X, X, -Y]$	$\left[0, \frac{3}{4}, \frac{7}{8}\right]$	[10,-22]
11	$[X, -X, -Y]$	$\left[0, \frac{3}{4}, \frac{7}{8}\right]$	[11,-23]
12	$[-X, -X, Y]$	$\left[0, \frac{1}{4}, \frac{5}{8}\right]$	[12,-21]

Table 20: Wyckoff bond: `24e@12d`

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

Table 21: Wyckoff bond: `24f@12d`

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

Table 22: Wyckoff bond: `48g@12d`

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

* Wyckoff site: `16e`, site symmetry: `.3.`

Table 23: Wyckoff bond: `16a@16e`

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]

Table 24: Wyckoff bond: `48b@16e`

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]
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]

* Wyckoff site: `24f`, site symmetry: `2..`

Table 25: Wyckoff bond: `24a@24f`

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]

Table 26: Wyckoff bond: `24b@24f`

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]

Table 27: Wyckoff bond: `48c@24f`

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]

* Wyckoff site: 24g, site symmetry: `..2`

Table 28: Wyckoff bond: `24a@24g`

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

Table 29: Wyckoff bond: `24b@24g`

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

Table 30: Wyckoff bond: `48c@24g`

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

Table 30

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

* Wyckoff site: `24h`, site symmetry: `..2`

Table 31: Wyckoff bond: `24a@24h`

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]

Table 32: Wyckoff bond: `24b@24h`

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]

Table 32

No.	vector	center	mapping
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]

Table 33: Wyckoff bond: `48c@24h`

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]
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]

* Wyckoff site: `48i`, site symmetry: `1`

Table 34: Wyckoff bond: `48a@48i`

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

Table 34

No.	vector	center	mapping
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]