SG No. 194 $\quad D_{6h}^4 \quad P6_3/mmc$ [hexagonal]

* plus set: $+[0, 0, 0]$

* Wyckoff site: 2a, site symmetry: -3m.

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 6b@2a

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

Table 3: Wyckoff bond: 6c@2a

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

Table 4: Wyckoff bond: 12d@2a

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

continued ...

1

Table 4

No.	vector	center	mapping
10	$[-Y, -X, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	[10,-22]
11	$[-X+Y, Y, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	[11,-23]
12	$[X, X-Y, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	[12,-24]

* Wyckoff site: 2b, site symmetry: -6m2

Table 5: Wyckoff bond: 2a@2b

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

Table 6: Wyckoff bond: 6b@2b

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

Table 7: Wyckoff bond: 6c@2b

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

Table 8: Wyckoff bond: 12d@2b

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[0, 0, \frac{1}{4}\right]$	[1,16]
2	$[-Y, X-Y, 0]$	$\left[0, 0, \frac{1}{4}\right]$	[2,17]
3	$[-X+Y, -X, 0]$	$\left[0, 0, \frac{1}{4}\right]$	[3,18]

continued ...

2

Table 8

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

Table 9: Wyckoff bond: `12e@2b`

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

Table 10: Wyckoff bond: `12f@2b`

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

Table 11: Wyckoff bond: `24g@2b`

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

* Wyckoff site: `2c`, site symmetry: `-6m2`

Table 12: Wyckoff bond: `2a@2c`

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

Table 13: Wyckoff bond: `6b@2c`

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

Table 14: Wyckoff bond: `6c@2c`

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

Table 15: Wyckoff bond: `12d@2c`

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

Table 16: Wyckoff bond: `12e@2c`

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

Table 17: Wyckoff bond: `12f@2c`

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

Table 18: Wyckoff bond: `24g@2c`

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

* Wyckoff site: `2d`, site symmetry: `-6m2`

Table 19: Wyckoff bond: `2a@2d`

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

Table 20: Wyckoff bond: `6b@2d`

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

Table 21: Wyckoff bond: `6c@2d`

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

Table 22: Wyckoff bond: `12d@2d`

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

Table 23: Wyckoff bond: `12e@2d`

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

Table 24: Wyckoff bond: `12f@2d`

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

Table 25: Wyckoff bond: `24g@2d`

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

continued ...

Table 25

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

* Wyckoff site: 4e, site symmetry: 3m.

Table 26: Wyckoff bond: 4a@4e

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

Table 27: Wyckoff bond: 12b@4e

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

Table 28: Wyckoff bond: `12c@4e`

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

Table 29: Wyckoff bond: `24d@4e`

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

* Wyckoff site: `4f`, site symmetry: `3m`.

Table 30: Wyckoff bond: `4a@4f`

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

Table 31: Wyckoff bond: `12b@4f`

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

Table 32: Wyckoff bond: `12c@4f`

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

Table 33: Wyckoff bond: `24d@4f`

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

* Wyckoff site: `6g`, site symmetry: `.2/m.`

Table 34: Wyckoff bond: `6a@6g`

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

Table 35: Wyckoff bond: `6b@6g`

No.	vector	center	mapping
1	$[X, 0, 0]$	$\left[\frac{1}{2}, 0, 0\right]$	[1,8,-13,-20]
2	$[0, X, 0]$	$\left[0, \frac{1}{2}, 0\right]$	[2,7,-14,-19]

continued ...

Table 35

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

Table 36: Wyckoff bond: `12c@6g`

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

* Wyckoff site: `6h`, site symmetry: `mm2`

Table 37: Wyckoff bond: `6a@6h`

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

Table 38: Wyckoff bond: `6b@6h`

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

Table 38

No.	vector	center	mapping
5	$[0, -X, 0]$	$\left[2x, x, \frac{3}{4}\right]$	[5,-7,14,-22]
6	$[X, X, 0]$	$\left[-x, x, \frac{3}{4}\right]$	[6,-9,15,-24]

Table 39: Wyckoff bond: `6c@6h`

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

Table 40: Wyckoff bond: `12d@6h`

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

Table 41: Wyckoff bond: `12e@6h`

No.	vector	center	mapping
1	$[X, 2X, Z]$	$\left[x, 2x, \frac{1}{4}\right]$	[1,20]
2	$[-2X, -X, Z]$	$\left[-2x, -x, \frac{1}{4}\right]$	[2,19]
3	$[X, -X, Z]$	$\left[x, -x, \frac{1}{4}\right]$	[3,21]
4	$[-X, -2X, Z]$	$\left[-x, -2x, \frac{3}{4}\right]$	[4,23]
5	$[2X, X, Z]$	$\left[2x, x, \frac{3}{4}\right]$	[5,22]
6	$[-X, X, Z]$	$\left[-x, x, \frac{3}{4}\right]$	[6,24]
7	$[2X, X, -Z]$	$\left[2x, x, \frac{3}{4}\right]$	[7,14]

continued ...

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Table 41

No.	vector	center	mapping
8	$[-X, -2X, -Z]$	$\left[-x, -2x, \frac{3}{4}\right]$	[8,13]
9	$[-X, X, -Z]$	$\left[-x, x, \frac{3}{4}\right]$	[9,15]
10	$[-2X, -X, -Z]$	$\left[-2x, -x, \frac{1}{4}\right]$	[10,17]
11	$[X, 2X, -Z]$	$\left[x, 2x, \frac{1}{4}\right]$	[11,16]
12	$[X, -X, -Z]$	$\left[x, -x, \frac{1}{4}\right]$	[12,18]

Table 42: Wyckoff bond: `12f@6h`

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

Table 43: Wyckoff bond: `24g@6h`

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

continued ...

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Table 43

No.	vector	center	mapping
18	$[-X+Y, -X, -Z]$	$[x, -x, \frac{1}{4}]$	[18]
19	$[-Y, -X, Z]$	$[-2x, -x, \frac{1}{4}]$	[19]
20	$[-X+Y, Y, Z]$	$[x, 2x, \frac{1}{4}]$	[20]
21	$[X, X-Y, Z]$	$[x, -x, \frac{1}{4}]$	[21]
22	$[Y, X, Z]$	$[2x, x, \frac{3}{4}]$	[22]
23	$[X-Y, -Y, Z]$	$[-x, -2x, \frac{3}{4}]$	[23]
24	$[-X, -X+Y, Z]$	$[-x, x, \frac{3}{4}]$	[24]

* Wyckoff site: `12i`, site symmetry: `.2.`

Table 44: Wyckoff bond: `12a@12i`

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

Table 45: Wyckoff bond: `12b@12i`

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

Table 46: Wyckoff bond: `24c@12i`

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

* Wyckoff site: `12j`, site symmetry: `m..`

Table 47: Wyckoff bond: `12a@12j`

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

Table 48: Wyckoff bond: `12b@12j`

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

Table 49: Wyckoff bond: `24c@12j`

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

* Wyckoff site: `12k`, site symmetry: `.m.`.

Table 50: Wyckoff bond: `12a@12k`

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

Table 51: Wyckoff bond: `12b@12k`

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

Table 52: Wyckoff bond: `24c@12k`

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

Table 52

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

* Wyckoff site: 24l, site symmetry: 1

Table 53: Wyckoff bond: 24a@24l

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