SG No. 204 T_{h}^5 $Im\bar{3}$ [cubic]

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

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

Table 1: Wyckoff bond: `6a@2a`

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

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

No.	vector	center	mapping
1	$[X, X, X]$	$[0, 0, 0]$	`[1,5,9,-13,-17,-21]`
2	$[-X, -X, X]$	$[0, 0, 0]$	`[2,7,12,-14,-19,-24]`
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: `12c@2a`

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

Table 4: Wyckoff bond: `24d@2a`

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

continued ...

Table 4

No.	vector	center	mapping
11	$[Y, -Z, -X]$	$[0, 0, 0]$	[11,-23]
12	$[-Y, -Z, X]$	$[0, 0, 0]$	[12,-24]

* Wyckoff site: `6b`, site symmetry: `mmm..`.

Table 5: Wyckoff bond: `6a@6b`

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

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

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

Table 7: Wyckoff bond: `6c@6b`

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

Table 8: Wyckoff bond: `12d@6b`

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

Table 9: Wyckoff bond: `12e@6b`

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

Table 10: Wyckoff bond: `12f@6b`

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

Table 11: Wyckoff bond: `24g@6b`

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

* Wyckoff site: `8c`, site symmetry: `.-3.`

Table 12: Wyckoff bond: `8a@8c`

No.	vector	center	mapping
1	$[X, X, X]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,5,9,-13,-17,-21]`

continued ...

Table 12

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

Table 13: Wyckoff bond: 24b@8c

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

* Wyckoff site: 12d, site symmetry: mm2..

Table 14: Wyckoff bond: 12a@12d

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

Table 15: Wyckoff bond: 12b@12d

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

continued ...

4

Table 15

No.	vector	center	mapping
6	$[0, X, 0]$	$[0, 0, -x]$	[10,-11,-21,24]

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

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

Table 17: Wyckoff bond: `24d@12d`

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

Table 18: Wyckoff bond: `24e@12d`

No.	vector	center	mapping
1	$[Y, 0, X]$	$[x, 0, 0]$	[1,15]
2	$[-Y, 0, X]$	$[-x, 0, 0]$	[2,16]
3	$[-Y, 0, -X]$	$[-x, 0, 0]$	[3,13]
4	$[Y, 0, -X]$	$[x, 0, 0]$	[4,14]
5	$[X, Y, 0]$	$[0, x, 0]$	[5,19]
6	$[X, -Y, 0]$	$[0, -x, 0]$	[6,20]
7	$[-X, -Y, 0]$	$[0, -x, 0]$	[7,17]
8	$[-X, Y, 0]$	$[0, x, 0]$	[8,18]

Table 18

No.	vector	center	mapping
9	$[0, X, Y]$	$[0, 0, x]$	[9,23]
10	$[0, X, -Y]$	$[0, 0, -x]$	[10,24]
11	$[0, -X, -Y]$	$[0, 0, -x]$	[11,21]
12	$[0, -X, Y]$	$[0, 0, x]$	[12,22]

Table 19: Wyckoff bond: 24f@12d

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

Table 20: Wyckoff bond: 48g@12d

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

continued ...

Table 20

No.	vector	center	mapping
19	$[Z, X, -Y]$	$[0, x, 0]$	[19]
20	$[Z, -X, Y]$	$[0, -x, 0]$	[20]
21	$[-Y, -Z, -X]$	$[0, 0, -x]$	[21]
22	$[Y, -Z, X]$	$[0, 0, x]$	[22]
23	$[-Y, Z, X]$	$[0, 0, x]$	[23]
24	$[Y, Z, -X]$	$[0, 0, -x]$	[24]

* Wyckoff site: 12e, site symmetry: mm2..

Table 21: Wyckoff bond: 12a@12e

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

Table 22: Wyckoff bond: 12b@12e

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

Table 23: Wyckoff bond: 12c@12e

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

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

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

Table 25: Wyckoff bond: `24e@12e`

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

Table 26: Wyckoff bond: `24f@12e`

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

Table 26

No.	vector	center	mapping
10	$[-Y, 0, X]$	$\left[\frac{1}{2}, x, 0\right]$	[18,-19]
11	$[-X, -Y, 0]$	$\left[0, \frac{1}{2}, -x\right]$	[21,-24]
12	$[X, -Y, 0]$	$\left[0, \frac{1}{2}, x\right]$	[22,-23]

Table 27: Wyckoff bond: `48g@12e`

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

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

Table 28: Wyckoff bond: `16a@16f`

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]

continued ...

Table 28

No.	vector	center	mapping
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 29: Wyckoff bond: 48b@16f

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

* Wyckoff site: 24g, site symmetry: m..

Table 30: Wyckoff bond: 24a@24g

No.	vector	center	mapping
1	$[0, X, Y]$	$[0, y, z]$	[1,16]
2	$[0, -X, Y]$	$[0, -y, z]$	[2,15]
3	$[0, X, -Y]$	$[0, y, -z]$	[3,14]
4	$[0, -X, -Y]$	$[0, -y, -z]$	[4,13]
5	$[Y, 0, X]$	$[z, 0, y]$	[5,20]

continued ...

Table 30

No.	vector	center	mapping
6	$[Y, 0, -X]$	$[z, 0, -y]$	[6,19]
7	$[-Y, 0, X]$	$[-z, 0, y]$	[7,18]
8	$[-Y, 0, -X]$	$[-z, 0, -y]$	[8,17]
9	$[X, Y, 0]$	$[y, z, 0]$	[9,24]
10	$[-X, Y, 0]$	$[-y, z, 0]$	[10,23]
11	$[X, -Y, 0]$	$[y, -z, 0]$	[11,22]
12	$[-X, -Y, 0]$	$[-y, -z, 0]$	[12,21]

Table 31: Wyckoff bond: 24b@24g

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

Table 32: Wyckoff bond: 48c@24g

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, z]$	[1]
2	$[-X, -Y, Z]$	$[0, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[0, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[0, -y, -z]$	[4]
5	$[Z, X, Y]$	$[z, 0, y]$	[5]
6	$[Z, -X, -Y]$	$[z, 0, -y]$	[6]
7	$[-Z, -X, Y]$	$[-z, 0, y]$	[7]
8	$[-Z, X, -Y]$	$[-z, 0, -y]$	[8]
9	$[Y, Z, X]$	$[y, z, 0]$	[9]
10	$[-Y, Z, -X]$	$[-y, z, 0]$	[10]
11	$[Y, -Z, -X]$	$[y, -z, 0]$	[11]
12	$[-Y, -Z, X]$	$[-y, -z, 0]$	[12]
13	$[-X, -Y, -Z]$	$[0, -y, -z]$	[13]
14	$[X, Y, -Z]$	$[0, y, -z]$	[14]
15	$[X, -Y, Z]$	$[0, -y, z]$	[15]

Table 32

No.	vector	center	mapping
16	$[-X, Y, Z]$	$[0, y, z]$	[16]
17	$[-Z, -X, -Y]$	$[-z, 0, -y]$	[17]
18	$[-Z, X, Y]$	$[-z, 0, y]$	[18]
19	$[Z, X, -Y]$	$[z, 0, -y]$	[19]
20	$[Z, -X, Y]$	$[z, 0, y]$	[20]
21	$[-Y, -Z, -X]$	$[-y, -z, 0]$	[21]
22	$[Y, -Z, X]$	$[y, -z, 0]$	[22]
23	$[-Y, Z, X]$	$[-y, z, 0]$	[23]
24	$[Y, Z, -X]$	$[y, z, 0]$	[24]

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

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

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