SG No. 217 T_{d}^3 $I\bar{4}3m$ [cubic]

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

* Wyckoff site: `2a`, site symmetry: `-43m`

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

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

Table 2: Wyckoff bond: `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	$[-X, X, -X]$	$[0, 0, 0]$	`[3,8,10,16,18,23]`
4	$[X, -X, -X]$	$[0, 0, 0]$	`[4,6,11,15,20,22]`

Table 3: Wyckoff bond: `12c@2a`

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

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

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

continued ...

1

Table 4

No.	vector	center	mapping
11	$[X, -Y, -X]$	$[0, 0, 0]$	[11,20]
12	$[-X, -Y, X]$	$[0, 0, 0]$	[12,19]

Table 5: Wyckoff bond: `24e@2a`

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

Table 6: Wyckoff bond: `48f@2a`

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

continued …

Table 6

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

* Wyckoff site: `6b`, site symmetry: `-42.m`

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

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

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

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

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

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

Table 10: Wyckoff bond: `24d@6b`

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

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

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

Table 12: Wyckoff bond: `24f@6b`

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

Table 12

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

Table 13: Wyckoff bond: `48g@6b`

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

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

Table 14: Wyckoff bond: `8a@8c`

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

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Table 15: Wyckoff bond: `24b@8c`

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

Table 16: Wyckoff bond: `24c@8c`

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

Table 17: Wyckoff bond: `48d@8c`

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]

Table 17

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

* Wyckoff site: `12d`, site symmetry: `-4..`

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

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

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

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

continued ...

Table 19

No.	vector	center	mapping
12	$[Y, -X, 0]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[22,-23]

Table 20: Wyckoff bond: `48c@12d`

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

* Wyckoff site: `12e`, site symmetry: `2.mm`

Table 21: Wyckoff bond: `12a@12e`

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

Table 22: Wyckoff bond: `12b@12e`

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

Table 23: Wyckoff bond: `24c@12e`

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

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

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

Table 25: Wyckoff bond: `48e@12e`

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

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

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

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

Table 27: Wyckoff bond: 24b@24f

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

Table 28: Wyckoff bond: 48c@24f

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

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

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

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

Table 30: Wyckoff bond: `24b@24g`

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

Table 31: Wyckoff bond: `48c@24g`

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

continued ...

Table 31

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

* Wyckoff site: 48h, site symmetry: 1

Table 32: 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	$[Y, X, Z]$	$[y, x, z]$	[13]
14	$[-Y, -X, Z]$	$[-y, -x, z]$	[14]
15	$[Y, -X, -Z]$	$[y, -x, -z]$	[15]
16	$[-Y, X, -Z]$	$[-y, x, -z]$	[16]
17	$[X, Z, Y]$	$[x, z, y]$	[17]
18	$[-X, Z, -Y]$	$[-x, z, -y]$	[18]
19	$[-X, -Z, Y]$	$[-x, -z, y]$	[19]
20	$[X, -Z, -Y]$	$[x, -z, -y]$	[20]
21	$[Z, Y, X]$	$[z, y, x]$	[21]
22	$[Z, -Y, -X]$	$[z, -y, -x]$	[22]
23	$[-Z, Y, -X]$	$[-z, y, -x]$	[23]
24	$[-Z, -Y, X]$	$[-z, -y, x]$	[24]