SG No. 200 T_h^1 $Pm\bar{3}$ [cubic]

* Wyckoff site: `1a`, site symmetry: `m-3`.

Table 1: Wyckoff bond: `3a@1a`

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: `4b@1a`

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: `6c@1a`

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: `12d@1a`

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: `1b`, site symmetry: `m-3`.

Table 5: Wyckoff bond: `3a@1b`

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

Table 6: Wyckoff bond: `4b@1b`

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

Table 7: Wyckoff bond: `6c@1b`

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

Table 8: Wyckoff bond: `12d@1b`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[1,-13]
2	$[-X, -Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[2,-14]
3	$[-X, Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[3,-15]
4	$[X, -Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[4,-16]
5	$[Z, X, Y]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[5,-17]

continued …

Table 8

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

* Wyckoff site: `3c`, site symmetry: `mmm..`

Table 9: Wyckoff bond: `3a@3c`

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 10: Wyckoff bond: `3b@3c`

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 11: Wyckoff bond: `3c@3c`

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 12: Wyckoff bond: `6d@3c`

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]

continued ...

Table 12

No.	vector	center	mapping
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 13: Wyckoff bond: `6e@3c`

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 14: Wyckoff bond: `6f@3c`

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 15: Wyckoff bond: `12g@3c`

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: 3d, site symmetry: mmm..

Table 16: Wyckoff bond: 3a@3d

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

Table 17: Wyckoff bond: 3b@3d

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

Table 18: Wyckoff bond: 3c@3d

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

Table 19: Wyckoff bond: 6d@3d

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

Table 20: Wyckoff bond: 6e@3d

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

continued …

Table 20

No.	vector	center	mapping
4	$[X, -Y, 0]$	$[0, \frac{1}{2}, 0]$	[6,-8,-18,20]
5	$[0, X, Y]$	$[0, 0, \frac{1}{2}]$	[9,-11,-21,23]
6	$[0, X, -Y]$	$[0, 0, \frac{1}{2}]$	[10,-12,-22,24]

Table 21: Wyckoff bond: `6f@3d`

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

Table 22: Wyckoff bond: `12g@3d`

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

* Wyckoff site: `6e`, site symmetry: `mm2..`

Table 23: Wyckoff bond: `6a@6e`

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]

continued ...

Table 23

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

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

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]
6	$[0, X, 0]$	$[0, 0, -x]$	[10,-11,-21,24]

Table 25: Wyckoff bond: `6c@6e`

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 26: Wyckoff bond: `12d@6e`

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 27: Wyckoff bond: `12e@6e`

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]`
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 28: Wyckoff bond: `12f@6e`

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 29: Wyckoff bond: `24g@6e`

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]`

continued ...

Table 29

No.	vector	center	mapping
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]
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: `6f`, site symmetry: `mm2..`

Table 30: Wyckoff bond: `6a@6f`

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 31: Wyckoff bond: `6b@6f`

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 32: Wyckoff bond: `6c@6f`

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 33: Wyckoff bond: `12d@6f`

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 34: Wyckoff bond: `12e@6f`

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 35: Wyckoff bond: `12f@6f`

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]
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 36: Wyckoff bond: `24g@6f`

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: `6g`, site symmetry: `mm2..`

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

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

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

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

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

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

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

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

continued ...

Table 40

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

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

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

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

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	$[0, -X, -Y]$	$\left[-x, \frac{1}{2}, 0\right]$	[13,-16]
8	$[0, X, -Y]$	$\left[x, \frac{1}{2}, 0\right]$	[14,-15]
9	$[-Y, 0, -X]$	$\left[0, -x, \frac{1}{2}\right]$	[17,-20]
10	$[-Y, 0, X]$	$\left[0, x, \frac{1}{2}\right]$	[18,-19]
11	$[-X, -Y, 0]$	$\left[\frac{1}{2}, 0, -x\right]$	[21,-24]
12	$[X, -Y, 0]$	$\left[\frac{1}{2}, 0, x\right]$	[22,-23]

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

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

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

Table 44: Wyckoff bond: `6a@6h`

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

Table 45: Wyckoff bond: `6b@6h`

No.	vector	center	mapping
1	$[0, 0, X]$	$[x, \frac{1}{2}, \frac{1}{2}]$	[1,-4,-14,15]
2	$[0, 0, X]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	[2,-3,-13,16]

continued ...

Table 45

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

Table 46: Wyckoff bond: `6c@6h`

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

Table 47: Wyckoff bond: `12d@6h`

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

Table 48: Wyckoff bond: `12e@6h`

No.	vector	center	mapping
1	$[Y, 0, X]$	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	[1,15]
2	$[-Y, 0, X]$	$\left[-x, \frac{1}{2}, \frac{1}{2}\right]$	[2,16]
3	$[-Y, 0, -X]$	$\left[-x, \frac{1}{2}, \frac{1}{2}\right]$	[3,13]
4	$[Y, 0, -X]$	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	[4,14]
5	$[X, Y, 0]$	$\left[\frac{1}{2}, x, \frac{1}{2}\right]$	[5,19]

continued ...

15

Table 48

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

Table 49: Wyckoff bond: 12f@6h

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

Table 50: Wyckoff bond: 24g@6h

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

continued …

Table 50

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

* Wyckoff site: `8i`, site symmetry: `.3.`

Table 51: Wyckoff bond: `8a@8i`

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

Table 52: Wyckoff bond: `24b@8i`

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]

Table 52

No.	vector	center	mapping
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: `12j`, site symmetry: `m..`

Table 53: Wyckoff bond: `12a@12j`

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]
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 54: Wyckoff bond: `12b@12j`

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]

continued ...

Table 54

No.	vector	center	mapping
12	$[0, 0, X]$	$[-y, -z, 0]$	[12,-21]

Table 55: Wyckoff bond: `24c@12j`

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]
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: `12k`, site symmetry: `m..`

Table 56: Wyckoff bond: `12a@12k`

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

continued ...

Table 56

No.	vector	center	mapping
8	$[-Y, 0, -X]$	$[-z, \frac{1}{2}, -y]$	[8,17]
9	$[X, Y, 0]$	$[y, z, \frac{1}{2}]$	[9,24]
10	$[-X, Y, 0]$	$[-y, z, \frac{1}{2}]$	[10,23]
11	$[X, -Y, 0]$	$[y, -z, \frac{1}{2}]$	[11,22]
12	$[-X, -Y, 0]$	$[-y, -z, \frac{1}{2}]$	[12,21]

Table 57: Wyckoff bond: `12b@12k`

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

Table 58: Wyckoff bond: `24c@12k`

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

continued ...

Table 58

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

* Wyckoff site: 24l, site symmetry: 1

Table 59: Wyckoff bond: 24a@24l

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]