SG No. 202 T_{h}^{3} $Fm\bar{3}$ [cubic]

* plus set: $+[0,\,0,\,0]$, $+\left[0,\,\frac{1}{2},\,\frac{1}{2}\right]$, $+\left[\frac{1}{2},\,0,\,\frac{1}{2}\right]$, $+\left[\frac{1}{2},\,\frac{1}{2},\,0\right]$
* Wyckoff site: `4a`, site symmetry: `m-3.`

Table 1: Wyckoff bond: `12a@4a`

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: `16b@4a`

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: `24c@4a`

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: `48d@4a`

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: `4b`, site symmetry: `m-3.`

Table 5: Wyckoff bond: `12a@4b`

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: `16b@4b`

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: `24c@4b`

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: `48d@4b`

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: 8c, site symmetry: 23.

Table 9: Wyckoff bond: 24a@8c

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

Table 10: Wyckoff bond: 32b@8c

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

Table 11: Wyckoff bond: 48c@8c

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,-2]
2	$[-X, Y, 0]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[3,-4]
3	$[0, X, Y]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[5,-6]
4	$[0, -X, Y]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[7,-8]
5	$[Y, 0, X]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[9,-10]

continued ...

Table 11

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

Table 12: Wyckoff bond: `96d@8c`

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

* Wyckoff site: `24d`, site symmetry: `2/m..`

Table 13: Wyckoff bond: `24a@24d`

No.	vector	center	mapping
1	$[0, X, Y]$	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	`[1,-4,-13,16]`

continued ...

Table 13

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

Table 14: Wyckoff bond: `24b@24d`

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

Table 15: Wyckoff bond: `48c@24d`

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

* Wyckoff site: `24e`, site symmetry: `mm2..`

Table 16: Wyckoff bond: `24a@24e`

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]`

continued ...

Table 16

No.	vector	center	mapping
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 17: Wyckoff bond: `24b@24e`

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 18: Wyckoff bond: `24c@24e`

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 19: Wyckoff bond: `48d@24e`

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 20: Wyckoff bond: `48e@24e`

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 21: Wyckoff bond: `48f@24e`

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 22: Wyckoff bond: `96g@24e`

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 22

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: `32f`, site symmetry: `.3.`

Table 23: Wyckoff bond: `32a@32f`

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 24: Wyckoff bond: `96b@32f`

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]`

continued ...

Table 24

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	$[-X, -Y, -Z]$	$[-x, -x, -x]$	`[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: `48g`, site symmetry: `2..`

Table 25: Wyckoff bond: `48a@48g`

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

Table 26: Wyckoff bond: `48b@48g`

No.	vector	center	mapping
1	$[X, 0, 0]$	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	`[1,4]`
2	$[-X, 0, 0]$	$\left[-x, \frac{3}{4}, \frac{1}{4}\right]$	`[2,3]`
3	$[0, X, 0]$	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	`[5,8]`
4	$[0, -X, 0]$	$\left[\frac{1}{4}, -x, \frac{3}{4}\right]$	`[6,7]`
5	$[0, 0, X]$	$\left[\frac{1}{4}, \frac{1}{4}, x\right]$	`[9,12]`

continued ...

Table 26

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

Table 27: Wyckoff bond: 96c@48g

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

* Wyckoff site: 48h, site symmetry: m..

Table 28: Wyckoff bond: 48a@48h

No.	vector	center	mapping
1	$[0, X, Y]$	$[0, y, z]$	[1,16]

continued ...

Table 28

No.	vector	center	mapping
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 29: Wyckoff bond: `48b@48h`

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 30: Wyckoff bond: `96c@48h`

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]`

continued ...

Table 30

No.	vector	center	mapping
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: 96i, site symmetry: 1

Table 31: Wyckoff bond: 96a@96i

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]