SG No. 134 D_{4h}^{12} $P4_2/nnm$ [tetragonal]

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

* Wyckoff site: `2a`, site symmetry: `-42m`

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

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

Table 2: Wyckoff bond: `4b@2a`

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

Table 3: Wyckoff bond: `4c@2a`

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

Table 4: Wyckoff bond: `8d@2a`

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

Table 5: Wyckoff bond: `8e@2a`

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

Table 6: Wyckoff bond: `8f@2a`

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

Table 7: Wyckoff bond: `16g@2a`

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

* Wyckoff site: 2b, site symmetry: -42m

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 4b@2b

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

Table 10: Wyckoff bond: 4c@2b

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

Table 11: Wyckoff bond: 8d@2b

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

Table 12: Wyckoff bond: `8e@2b`

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

Table 13: Wyckoff bond: `8f@2b`

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

Table 14: Wyckoff bond: `16g@2b`

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

* Wyckoff site: `4c`, site symmetry: `222`.

Table 15: Wyckoff bond: `4a@4c`

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

Table 16: Wyckoff bond: `4b@4c`

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

Table 17: Wyckoff bond: `4c@4c`

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

Table 18: Wyckoff bond: `8d@4c`

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

Table 19: Wyckoff bond: `8e@4c`

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

Table 20: Wyckoff bond: `8f@4c`

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

Table 21: Wyckoff bond: `16g@4c`

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	$[-Y, X, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[3]`
4	$[Y, -X, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[4]`
5	$[-X, Y, -Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[5]`
6	$[X, -Y, -Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[6]`
7	$[Y, X, -Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[7]`
8	$[-Y, -X, -Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[8]`
9	$[-X, -Y, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[9]`
10	$[X, Y, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[10]`
11	$[Y, -X, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[11]`
12	$[-Y, X, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[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	$[-Y, -X, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[15]`
16	$[Y, X, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[16]`

* Wyckoff site: 4d, site symmetry: 2.22

Table 22: Wyckoff bond: 4a@4d

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

Table 23: Wyckoff bond: 4b@4d

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

Table 24: Wyckoff bond: 4c@4d

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

Table 25: Wyckoff bond: 8d@4d

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

Table 26: Wyckoff bond: `8e@4d`

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

Table 27: Wyckoff bond: `8f@4d`

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

Table 28: Wyckoff bond: `16g@4d`

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

* Wyckoff site: `4e`, site symmetry: `..2/m`

Table 29: Wyckoff bond: `4a@4e`

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

Table 30: Wyckoff bond: `4b@4e`

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

Table 31: Wyckoff bond: `8c@4e`

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

* Wyckoff site: `4f`, site symmetry: `..2/m`

Table 32: Wyckoff bond: `4a@4f`

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

Table 33: Wyckoff bond: `4b@4f`

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

Table 34: Wyckoff bond: `8c@4f`

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

* Wyckoff site: `4g`, site symmetry: `2.mm`

Table 35: Wyckoff bond: `4a@4g`

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

Table 36: Wyckoff bond: `4b@4g`

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

Table 37: Wyckoff bond: `8c@4g`

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

Table 38: Wyckoff bond: `8d@4g`

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

Table 39: Wyckoff bond: `16e@4g`

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

Table 40: Wyckoff bond: 8a@8h

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

Table 41: Wyckoff bond: 8b@8h

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

Table 42: Wyckoff bond: 16c@8h

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

continued ...

Table 42

No.	vector	center	mapping
16	$[Y, X, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, z\right]$	[16]

* Wyckoff site: `8i`, site symmetry: `.2.`

Table 43: Wyckoff bond: `8a@8i`

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

Table 44: Wyckoff bond: `8b@8i`

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

Table 45: Wyckoff bond: `16c@8i`

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

Table 45

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

* Wyckoff site: 8j, site symmetry: .2.

Table 46: Wyckoff bond: 8a@8j

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

Table 47: Wyckoff bond: 8b@8j

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

Table 48: Wyckoff bond: 16c@8j

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	[1]
2	$[-X, -Y, Z]$	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}\right]$	[2]
3	$[-Y, X, Z]$	$\left[\frac{1}{4}, x, \frac{3}{4}\right]$	[3]

continued ...

Table 48

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

* Wyckoff site: `8k`, site symmetry: `..2`

Table 49: Wyckoff bond: `8a@8k`

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

Table 50: Wyckoff bond: `8b@8k`

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

Table 51: Wyckoff bond: `16c@8k`

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

* Wyckoff site: `8l`, site symmetry: `..2`

Table 52: Wyckoff bond: `8a@8l`

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

Table 53: Wyckoff bond: `8b@8l`

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

Table 54: Wyckoff bond: 16c@8l

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

* Wyckoff site: 8m, site symmetry: ..m

Table 55: Wyckoff bond: 8a@8m

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

Table 56: Wyckoff bond: 8b@8m

No.	vector	center	mapping
1	$[X, X, 0]$	$[x, -x, z]$	[1,-15]
2	$[-X, -X, 0]$	$\left[\frac{1}{2} - x, x + \frac{1}{2}, z\right]$	[2,-16]
3	$[-X, X, 0]$	$\left[x + \frac{1}{2}, x, z + \frac{1}{2}\right]$	[3,-13]
4	$[X, -X, 0]$	$\left[-x, \frac{1}{2} - x, z + \frac{1}{2}\right]$	[4,-14]
5	$[-X, X, 0]$	$\left[\frac{1}{2} - x, -x, \frac{1}{2} - z\right]$	[5,-11]
6	$[X, -X, 0]$	$\left[x, x + \frac{1}{2}, \frac{1}{2} - z\right]$	[6,-12]

continued …

Table 56

No.	vector	center	mapping
7	$[X, X, 0]$	$[-x, x, -z]$	[7,-9]
8	$[-X, -X, 0]$	$\left[x + \frac{1}{2}, \frac{1}{2} - x, -z\right]$	[8,-10]

Table 57: Wyckoff bond: `16c@8m`

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

* Wyckoff site: `16n`, site symmetry: `1`

Table 58: Wyckoff bond: `16a@16n`

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

continued ...

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Table 58

No.	vector	center	mapping
15	$[-Y,\, -X,\, Z]$	$[-y,\, -x,\, z]$	[15]
16	$[Y,\, X,\, Z]$	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	[16]

No.	vector	center	mapping
15	$[-Y,\, -X,\, Z]$	$[-y,\, -x,\, z]$	[15]
16	$[Y,\, X,\, Z]$	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	[16]