SG No. 126 D_{4h}^4 $P4/nnc$ [tetragonal]

Table 1: Wyckoff bond: 2a@2a

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

Table 2: Wyckoff bond: 4b@2a

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

Table 3: Wyckoff bond: 4c@2a

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

Table 4: Wyckoff bond: 8d@2a

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	$[0, X, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[3,-8]
4	$[0, -X, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[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	$[0, -X, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[11,-16]
8	$[0, X, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[12,-15]

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

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

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

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

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

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

* Wyckoff site: 2b, site symmetry: 422

Table 8: Wyckoff bond: 2a@2b

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

Table 9: Wyckoff bond: 4b@2b

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

Table 10: Wyckoff bond: 4c@2b

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

Table 11: Wyckoff bond: 8d@2b

No.	vector	center	mapping
1	$[X, 0, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[1,-5]
2	$[-X, 0, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[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	$[-X, 0, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[9,-13]
6	$[X, 0, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[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 12: Wyckoff bond: `8e@2b`

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

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

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

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

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[1]
2	$[-X, -Y, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[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	$[-X, Y, -Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[5]
6	$[X, -Y, -Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[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	$[-X, -Y, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[9]
10	$[X, Y, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[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	$[X, -Y, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[13]
14	$[-X, Y, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[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: `4c`, site symmetry: `222`.

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

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

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

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

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

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

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

No.	vector	center	mapping
1	$[X, 0, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[1,-5]`
2	$[-X, 0, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[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	$[-X, 0, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[9,-13]`
6	$[X, 0, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[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 19: Wyckoff bond: `8e@4c`

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

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

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

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

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[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	$[-X, Y, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[5]`
6	$[X, -Y, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[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	$[-X, -Y, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[9]`
10	$[X, Y, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[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	$[X, -Y, Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[13]`
14	$[-X, Y, Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[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: 4d, site symmetry: -4..

Table 22: Wyckoff bond: 4a@4d

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

Table 23: Wyckoff bond: 8b@4d

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

Table 24: Wyckoff bond: 16c@4d

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

* Wyckoff site: 4e, site symmetry: 4..

Table 25: Wyckoff bond: `4a@4e`

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

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

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

Table 27: Wyckoff bond: `16c@4e`

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	$[-Y, X, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	[3]
4	$[Y, -X, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	[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	$[Y, X, -Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}-z\right]$	[7]
8	$[-Y, -X, -Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}-z\right]$	[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	$[Y, -X, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[11]
12	$[-Y, X, -Z]$	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[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	$[-Y, -X, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, z+\frac{1}{2}\right]$	[15]
16	$[Y, X, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, z+\frac{1}{2}\right]$	[16]

* Wyckoff site: `8f`, site symmetry: `-1`

Table 28: Wyckoff bond: `8a@8f`

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	$[-Y, X, Z]$	$\left[\frac{1}{2}, 0, 0\right]$	[3,-11]
4	$[Y, -X, Z]$	$\left[0, \frac{1}{2}, 0\right]$	[4,-12]
5	$[-X, Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[5,-13]
6	$[X, -Y, -Z]$	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[6,-14]
7	$[Y, X, -Z]$	$\left[0, 0, \frac{1}{2}\right]$	[7,-15]
8	$[-Y, -X, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[8,-16]

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

Table 29: Wyckoff bond: `8a@8g`

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

Table 30: Wyckoff bond: `8b@8g`

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

Table 31: Wyckoff bond: `16c@8g`

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

continued …

Table 31

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

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

Table 32: Wyckoff bond: `8a@8h`

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

Table 33: Wyckoff bond: `8b@8h`

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

Table 34: Wyckoff bond: `16c@8h`

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

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

Table 35: Wyckoff bond: `8a@8i`

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	$[-X, 0, Z]$	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[3,-7]
4	$[X, 0, Z]$	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}\right]$	[4,-8]
5	$[0, -X, -Z]$	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	[9,-14]
6	$[0, X, -Z]$	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[10,-13]
7	$[X, 0, -Z]$	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[11,-15]
8	$[-X, 0, -Z]$	$\left[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}\right]$	[12,-16]

Table 36: Wyckoff bond: `8b@8i`

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	$[0, X, 0]$	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[3,7]
4	$[0, -X, 0]$	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}\right]$	[4,8]
5	$[-X, 0, 0]$	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	[9,14]
6	$[X, 0, 0]$	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[10,13]
7	$[0, -X, 0]$	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[11,15]
8	$[0, X, 0]$	$\left[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}\right]$	[12,16]

Table 37: Wyckoff bond: 16c@8i

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	$[-Y, X, Z]$	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[3]
4	$[Y, -X, Z]$	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}\right]$	[4]
5	$[-X, Y, -Z]$	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}\right]$	[5]
6	$[X, -Y, -Z]$	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	[6]
7	$[Y, X, -Z]$	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[7]
8	$[-Y, -X, -Z]$	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}\right]$	[8]
9	$[-X, -Y, -Z]$	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	[9]
10	$[X, Y, -Z]$	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[10]
11	$[Y, -X, -Z]$	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[11]
12	$[-Y, X, -Z]$	$\left[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}\right]$	[12]
13	$[X, -Y, Z]$	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[13]
14	$[-X, Y, Z]$	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	[14]
15	$[-Y, -X, Z]$	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[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 38: Wyckoff bond: 8a@8j

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

Table 39: Wyckoff bond: 8b@8j

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

continued ...

Table 39

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

Table 40: Wyckoff bond: `16c@8j`

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

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

Table 41: Wyckoff bond: `16a@16k`

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	$[-Y, X, Z]$	$\left[\frac{1}{2}-y, x, z\right]$	[3]
4	$[Y, -X, Z]$	$\left[y, \frac{1}{2}-x, z\right]$	[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	$[Y, X, -Z]$	$\left[y, x, \frac{1}{2}-z\right]$	[7]
8	$[-Y, -X, -Z]$	$\left[\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[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	$[Y, -X, -Z]$	$\left[y+\frac{1}{2}, -x, -z\right]$	[11]
12	$[-Y, X, -Z]$	$\left[-y, x+\frac{1}{2}, -z\right]$	[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 ...

Table 41

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

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