SG No. 130 $D_{4\mathrm{h}}^8$ $P4/ncc$ [tetragonal]

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

* Wyckoff site: `4a`, site symmetry: `2.22`

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

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

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

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

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

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

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

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

Table 5: Wyckoff bond: `8e@4a`

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

Table 6: Wyckoff bond: `8f@4a`

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

Table 7: Wyckoff bond: `16g@4a`

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

* Wyckoff site: 4b, site symmetry: -4..

Table 8: Wyckoff bond: 4a@4b

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[1,2,-11,-12]
2	$[0, 0, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[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 9: Wyckoff bond: 8b@4b

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[1,-2]
2	$[-Y, X, 0]$	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[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	$[-X, -Y, 0]$	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[9,-10]
6	$[Y, -X, 0]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[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 10: Wyckoff bond: 16c@4b

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[1]
2	$[-X, -Y, Z]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[2]
3	$[-Y, X, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[3]
4	$[Y, -X, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[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	$[-X, -Y, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[9]
10	$[X, Y, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[10]
11	$[Y, -X, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[11]
12	$[-Y, X, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[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: 4c, site symmetry: 4..

Table 11: Wyckoff bond: `4a@4c`

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

Table 12: Wyckoff bond: `8b@4c`

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

Table 13: Wyckoff bond: `16c@4c`

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

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

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

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

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

Table 15: Wyckoff bond: `8a@8e`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	[1,-2]
2	$[-Y, X, 0]$	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[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	$[-X, -Y, 0]$	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	[9,-10]
6	$[Y, -X, 0]$	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[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 16: Wyckoff bond: `8b@8e`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	[1,2]
2	$[0, 0, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[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	$[0, 0, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	[9,10]
6	$[0, 0, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[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 17: Wyckoff bond: `16c@8e`

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

continued ...

Table 17

No.	vector	center	mapping
2	$[-X, -Y, Z]$	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	[2]
3	$[-Y, X, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[3]
4	$[Y, -X, Z]$	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[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	$[-X, -Y, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	[9]
10	$[X, Y, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	[10]
11	$[Y, -X, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[11]
12	$[-Y, X, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[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: `8f`, site symmetry: `..2`

Table 18: Wyckoff bond: `8a@8f`

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

Table 19: Wyckoff bond: `8b@8f`

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

Table 20: Wyckoff bond: `16c@8f`

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

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

Table 21: Wyckoff bond: `16a@16g`

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	$[-X, Y, -Z]$	$\left[-x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[5]
6	$[X, -Y, -Z]$	$\left[x + \frac{1}{2}, -y, \frac{1}{2} - z\right]$	[6]
7	$[Y, X, -Z]$	$\left[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z\right]$	[7]
8	$[-Y, -X, -Z]$	$\left[-y, -x, \frac{1}{2} - z\right]$	[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	$[-X, Y, Z]$	$\left[\frac{1}{2} - x, y, z + \frac{1}{2}\right]$	[14]
15	$[-Y, -X, Z]$	$\left[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}\right]$	[15]
16	$[Y, X, Z]$	$\left[y, x, z + \frac{1}{2}\right]$	[16]