SG No. 139 D_{4h}^{17} $I4/mmm$ [tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

* Wyckoff site: `2b`, site symmetry: `4/mmm`

Table 8: Wyckoff bond: `2a@2b`

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

Table 9: Wyckoff bond: `4b@2b`

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

Table 10: Wyckoff bond: `4c@2b`

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

Table 11: Wyckoff bond: `8d@2b`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

* Wyckoff site: `4d`, site symmetry: `-4m2`

Table 22: Wyckoff bond: `4a@4d`

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

Table 23: Wyckoff bond: `8b@4d`

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

Table 24: Wyckoff bond: `8c@4d`

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

continued ...

Table 24

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

Table 25: Wyckoff bond: `16d@4d`

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

Table 26: Wyckoff bond: `16e@4d`

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

Table 27: Wyckoff bond: `16f@4d`

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

Table 28: Wyckoff bond: `32g@4d`

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

* Wyckoff site: `4e`, site symmetry: `4mm`

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

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

Table 30: Wyckoff bond: `8b@4e`

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

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

No.	vector	center	mapping
1	$[X, X, 0]$	$[0, 0, z]$	`[1,-2,-15,16]`
2	$[-X, X, 0]$	$[0, 0, z]$	`[3,-4,-13,14]`
3	$[-X, X, 0]$	$[0, 0, -z]$	`[5,-6,-11,12]`

continued ...

Table 31

No.	vector	center	mapping
4	$[X, X, 0]$	$[0, 0, -z]$	`[7,-8,-9,10]`

Table 32: Wyckoff bond: `16d@4e`

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

Table 33: Wyckoff bond: `16e@4e`

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

Table 34: Wyckoff bond: `16f@4e`

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

Table 35: Wyckoff bond: `32g@4e`

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

* Wyckoff site: `8f`, site symmetry: `..2/m`

Table 36: Wyckoff bond: `8a@8f`

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

Table 37: Wyckoff bond: `8b@8f`

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

Table 38: Wyckoff bond: `16c@8f`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,-9]`

continued ...

Table 38

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

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

Table 39: Wyckoff bond: `8a@8g`

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

Table 40: Wyckoff bond: `8b@8g`

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

Table 41: Wyckoff bond: `16c@8g`

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

Table 42: Wyckoff bond: `16d@8g`

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

Table 43: Wyckoff bond: `32e@8g`

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

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

Table 44: Wyckoff bond: `8a@8h`

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

Table 45: Wyckoff bond: `8b@8h`

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

Table 46: Wyckoff bond: `8c@8h`

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

Table 47: Wyckoff bond: `16d@8h`

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

Table 48: Wyckoff bond: `16e@8h`

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

Table 49: Wyckoff bond: `16f@8h`

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

Table 50: Wyckoff bond: `32g@8h`

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

* Wyckoff site: `8i`, site symmetry: `m2m.`

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

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

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

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

Table 53: Wyckoff bond: `8c@8i`

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

Table 54: Wyckoff bond: `16d@8i`

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

Table 55: Wyckoff bond: `16e@8i`

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

Table 56: Wyckoff bond: `16f@8i`

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

Table 57: Wyckoff bond: `32g@8i`

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

* Wyckoff site: `8j`, site symmetry: `m2m.`

Table 58: Wyckoff bond: `8a@8j`

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

Table 59: Wyckoff bond: `8b@8j`

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

Table 60: Wyckoff bond: `8c@8j`

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

Table 61: Wyckoff bond: `16d@8j`

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

Table 62: Wyckoff bond: `16e@8j`

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

Table 63: Wyckoff bond: `16f@8j`

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

Table 64: Wyckoff bond: `32g@8j`

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

* Wyckoff site: `16k`, site symmetry: `..2`

Table 65: Wyckoff bond: `16a@16k`

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

Table 66: Wyckoff bond: `16b@16k`

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

Table 67: Wyckoff bond: `32c@16k`

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

* Wyckoff site: `16l`, site symmetry: `m..`

Table 68: Wyckoff bond: `16a@16l`

No.	vector	center	mapping
1	$[X,\ Y,\ 0]$	$[x,\ y,\ 0]$	`[1,10]`
2	$[-X,\ -Y,\ 0]$	$[-x,\ -y,\ 0]$	`[2,9]`
3	$[-Y,\ X,\ 0]$	$[-y,\ x,\ 0]$	`[3,12]`
4	$[Y,\ -X,\ 0]$	$[y,\ -x,\ 0]$	`[4,11]`
5	$[-X,\ Y,\ 0]$	$[-x,\ y,\ 0]$	`[5,14]`
6	$[X,\ -Y,\ 0]$	$[x,\ -y,\ 0]$	`[6,13]`

continued ...

Table 68

No.	vector	center	mapping
7	$[Y, X, 0]$	$[y, x, 0]$	[7,16]
8	$[-Y, -X, 0]$	$[-y, -x, 0]$	[8,15]

Table 69: Wyckoff bond: 16b@16l

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, y, 0]$	[1,-10]
2	$[0, 0, Z]$	$[-x, -y, 0]$	[2,-9]
3	$[0, 0, Z]$	$[-y, x, 0]$	[3,-12]
4	$[0, 0, Z]$	$[y, -x, 0]$	[4,-11]
5	$[0, 0, -Z]$	$[-x, y, 0]$	[5,-14]
6	$[0, 0, -Z]$	$[x, -y, 0]$	[6,-13]
7	$[0, 0, -Z]$	$[y, x, 0]$	[7,-16]
8	$[0, 0, -Z]$	$[-y, -x, 0]$	[8,-15]

Table 70: Wyckoff bond: 32c@16l

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, 0]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, 0]$	[2]
3	$[-Y, X, Z]$	$[-y, x, 0]$	[3]
4	$[Y, -X, Z]$	$[y, -x, 0]$	[4]
5	$[-X, Y, -Z]$	$[-x, y, 0]$	[5]
6	$[X, -Y, -Z]$	$[x, -y, 0]$	[6]
7	$[Y, X, -Z]$	$[y, x, 0]$	[7]
8	$[-Y, -X, -Z]$	$[-y, -x, 0]$	[8]
9	$[-X, -Y, -Z]$	$[-x, -y, 0]$	[9]
10	$[X, Y, -Z]$	$[x, y, 0]$	[10]
11	$[Y, -X, -Z]$	$[y, -x, 0]$	[11]
12	$[-Y, X, -Z]$	$[-y, x, 0]$	[12]
13	$[X, -Y, Z]$	$[x, -y, 0]$	[13]
14	$[-X, Y, Z]$	$[-x, y, 0]$	[14]
15	$[-Y, -X, Z]$	$[-y, -x, 0]$	[15]
16	$[Y, X, Z]$	$[y, x, 0]$	[16]

* Wyckoff site: 16m, site symmetry: ..m

Table 71: Wyckoff bond: `16a@16m`

No.	vector	center	mapping
1	$[X, X, Z]$	$[x, x, z]$	`[1,16]`
2	$[-X, -X, Z]$	$[-x, -x, z]$	`[2,15]`
3	$[-X, X, Z]$	$[-x, x, z]$	`[3,14]`
4	$[X, -X, Z]$	$[x, -x, z]$	`[4,13]`
5	$[-X, X, -Z]$	$[-x, x, -z]$	`[5,12]`
6	$[X, -X, -Z]$	$[x, -x, -z]$	`[6,11]`
7	$[X, X, -Z]$	$[x, x, -z]$	`[7,10]`
8	$[-X, -X, -Z]$	$[-x, -x, -z]$	`[8,9]`

Table 72: Wyckoff bond: `16b@16m`

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, x, z]$	`[1,-16]`
2	$[-X, X, 0]$	$[-x, -x, z]$	`[2,-15]`
3	$[X, X, 0]$	$[-x, x, z]$	`[3,-14]`
4	$[-X, -X, 0]$	$[x, -x, z]$	`[4,-13]`
5	$[-X, -X, 0]$	$[-x, x, -z]$	`[5,-12]`
6	$[X, X, 0]$	$[x, -x, -z]$	`[6,-11]`
7	$[-X, X, 0]$	$[x, x, -z]$	`[7,-10]`
8	$[X, -X, 0]$	$[-x, -x, -z]$	`[8,-9]`

Table 73: Wyckoff bond: `32c@16m`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, x, z]$	`[1]`
2	$[-X, -Y, Z]$	$[-x, -x, z]$	`[2]`
3	$[-Y, X, Z]$	$[-x, x, z]$	`[3]`
4	$[Y, -X, Z]$	$[x, -x, z]$	`[4]`
5	$[-X, Y, -Z]$	$[-x, x, -z]$	`[5]`
6	$[X, -Y, -Z]$	$[x, -x, -z]$	`[6]`
7	$[Y, X, -Z]$	$[x, x, -z]$	`[7]`
8	$[-Y, -X, -Z]$	$[-x, -x, -z]$	`[8]`
9	$[-X, -Y, -Z]$	$[-x, -x, -z]$	`[9]`
10	$[X, Y, -Z]$	$[x, x, -z]$	`[10]`
11	$[Y, -X, -Z]$	$[x, -x, -z]$	`[11]`
12	$[-Y, X, -Z]$	$[-x, x, -z]$	`[12]`
13	$[X, -Y, Z]$	$[x, -x, z]$	`[13]`
14	$[-X, Y, Z]$	$[-x, x, z]$	`[14]`
15	$[-Y, -X, Z]$	$[-x, -x, z]$	`[15]`
16	$[Y, X, Z]$	$[x, x, z]$	`[16]`

* Wyckoff site: 16n, site symmetry: .m.

Table 74: Wyckoff bond: 16a@16n

No.	vector	center	mapping
1	$[0, X, Z]$	$[0, y, z]$	[1,14]
2	$[0, -X, Z]$	$[0, -y, z]$	[2,13]
3	$[-X, 0, Z]$	$[-y, 0, z]$	[3,15]
4	$[X, 0, Z]$	$[y, 0, z]$	[4,16]
5	$[0, X, -Z]$	$[0, y, -z]$	[5,10]
6	$[0, -X, -Z]$	$[0, -y, -z]$	[6,9]
7	$[X, 0, -Z]$	$[y, 0, -z]$	[7,11]
8	$[-X, 0, -Z]$	$[-y, 0, -z]$	[8,12]

Table 75: Wyckoff bond: 16b@16n

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	[1,-14]
2	$[-X, 0, 0]$	$[0, -y, z]$	[2,-13]
3	$[0, X, 0]$	$[-y, 0, z]$	[3,-15]
4	$[0, -X, 0]$	$[y, 0, z]$	[4,-16]
5	$[-X, 0, 0]$	$[0, y, -z]$	[5,-10]
6	$[X, 0, 0]$	$[0, -y, -z]$	[6,-9]
7	$[0, X, 0]$	$[y, 0, -z]$	[7,-11]
8	$[0, -X, 0]$	$[-y, 0, -z]$	[8,-12]

Table 76: Wyckoff bond: 32c@16n

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, z]$	[1]
2	$[-X, -Y, Z]$	$[0, -y, z]$	[2]
3	$[-Y, X, Z]$	$[-y, 0, z]$	[3]
4	$[Y, -X, Z]$	$[y, 0, z]$	[4]
5	$[-X, Y, -Z]$	$[0, y, -z]$	[5]
6	$[X, -Y, -Z]$	$[0, -y, -z]$	[6]
7	$[Y, X, -Z]$	$[y, 0, -z]$	[7]
8	$[-Y, -X, -Z]$	$[-y, 0, -z]$	[8]
9	$[-X, -Y, -Z]$	$[0, -y, -z]$	[9]
10	$[X, Y, -Z]$	$[0, y, -z]$	[10]
11	$[Y, -X, -Z]$	$[y, 0, -z]$	[11]
12	$[-Y, X, -Z]$	$[-y, 0, -z]$	[12]
13	$[X, -Y, Z]$	$[0, -y, z]$	[13]
14	$[-X, Y, Z]$	$[0, y, z]$	[14]
15	$[-Y, -X, Z]$	$[-y, 0, z]$	[15]

continued ...

Table 76

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

* Wyckoff site: 32o, site symmetry: 1

Table 77: Wyckoff bond: 32a@32o

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