SG No. 123 D_{4h}^1 $P4/mmm$ [tetragonal]

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

* Wyckoff site: `1a`, site symmetry: `4/mmm`

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

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: `2b@1a`

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: `2c@1a`

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: `4d@1a`

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: `4e@1a`

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: `4f@1a`

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: `8g@1a`

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: `1b`, site symmetry: `4/mmm`

Table 8: Wyckoff bond: `1a@1b`

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: `2b@1b`

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: `2c@1b`

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: `4d@1b`

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

Table 12: Wyckoff bond: `4e@1b`

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

Table 13: Wyckoff bond: `4f@1b`

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

Table 14: Wyckoff bond: `8g@1b`

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

* Wyckoff site: `1c`, site symmetry: `4/mmm`

Table 15: Wyckoff bond: `1a@1c`

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

Table 16: Wyckoff bond: `2b@1c`

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

Table 17: Wyckoff bond: `2c@1c`

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

Table 18: Wyckoff bond: `4d@1c`

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

Table 19: Wyckoff bond: `4e@1c`

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

Table 20: Wyckoff bond: `4f@1c`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[1,-2,-9,10]`

continued …

Table 20

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

Table 21: Wyckoff bond: 8g@1c

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

* Wyckoff site: 1d, site symmetry: 4/mmm

Table 22: Wyckoff bond: 1a@1d

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

Table 23: Wyckoff bond: 2b@1d

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

Table 24: Wyckoff bond: 2c@1d

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

Table 25: Wyckoff bond: `4d@1d`

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

Table 26: Wyckoff bond: `4e@1d`

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

Table 27: Wyckoff bond: `4f@1d`

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

Table 28: Wyckoff bond: `8g@1d`

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

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

Table 29: Wyckoff bond: `2a@2e`

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

Table 30: Wyckoff bond: `2b@2e`

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

Table 31: Wyckoff bond: `2c@2e`

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

Table 32: Wyckoff bond: `4d@2e`

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

Table 33: Wyckoff bond: `4e@2e`

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

Table 34: Wyckoff bond: `4f@2e`

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

Table 35: Wyckoff bond: `8g@2e`

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

* Wyckoff site: `2f`, site symmetry: `mmm`.

Table 36: Wyckoff bond: `2a@2f`

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 37: Wyckoff bond: `2b@2f`

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 38: Wyckoff bond: `2c@2f`

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 39: Wyckoff bond: `4d@2f`

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

Table 40: Wyckoff bond: `4e@2f`

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

Table 41: Wyckoff bond: `4f@2f`

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

Table 42: Wyckoff bond: `8g@2f`

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

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

Table 43: Wyckoff bond: **2a@2g**

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 44: Wyckoff bond: **4b@2g**

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 45: Wyckoff bond: **4c@2g**

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]
4	$[X, X, 0]$	$[0, 0, -z]$	[7,-8,-9,10]

Table 46: Wyckoff bond: **8d@2g**

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 47: Wyckoff bond: **8e@2g**

No.	vector	center	mapping
1	$[X, X, Z]$	$[0, 0, z]$	[1,16]
2	$[-X, -X, Z]$	$[0, 0, z]$	[2,15]

continued ...

Table 47

No.	vector	center	mapping
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 48: Wyckoff bond: `8f@2g`

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 49: Wyckoff bond: `16g@2g`

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: `2h`, site symmetry: `4mm`

Table 50: Wyckoff bond: **2a@2h**

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

Table 51: Wyckoff bond: **4b@2h**

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

Table 52: Wyckoff bond: **4c@2h**

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

Table 53: Wyckoff bond: **8d@2h**

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

Table 54: Wyckoff bond: **8e@2h**

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

continued ...

Table 54

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

Table 55: Wyckoff bond: 8f@2h

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

Table 56: Wyckoff bond: 16g@2h

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

* Wyckoff site: 4i, site symmetry: 2mm.

Table 57: Wyckoff bond: `4a@4i`

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 58: Wyckoff bond: `4b@4i`

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

Table 59: Wyckoff bond: `4c@4i`

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 60: Wyckoff bond: `8d@4i`

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 61: Wyckoff bond: `8e@4i`

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

Table 62: Wyckoff bond: `8f@4i`

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 63: Wyckoff bond: `16g@4i`

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: 4j, site symmetry: m.2m

Table 64: Wyckoff bond: 4a@4j

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 65: Wyckoff bond: 4b@4j

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 66: Wyckoff bond: 4c@4j

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 67: Wyckoff bond: 8d@4j

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 68: Wyckoff bond: `8e@4j`

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 69: Wyckoff bond: `8f@4j`

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 70: Wyckoff bond: `16g@4j`

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: 4k, site symmetry: `m.2m`

Table 71: Wyckoff bond: `4a@4k`

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

Table 72: Wyckoff bond: `4b@4k`

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

Table 73: Wyckoff bond: `4c@4k`

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

Table 74: Wyckoff bond: `8d@4k`

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

Table 75: Wyckoff bond: `8e@4k`

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

Table 76: Wyckoff bond: `8f@4k`

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

Table 77: Wyckoff bond: `16g@4k`

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

* Wyckoff site: 4l, site symmetry: m2m.

Table 78: Wyckoff bond: 4a@4l

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 79: Wyckoff bond: 4b@4l

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 80: Wyckoff bond: 4c@4l

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 81: Wyckoff bond: 8d@4l

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 82: Wyckoff bond: 8e@4l

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 83: Wyckoff bond: 8f@4l

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 84: Wyckoff bond: 16g@4l

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: 4m, site symmetry: m2m.

Table 85: Wyckoff bond: 4a@4m

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

Table 86: Wyckoff bond: 4b@4m

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

Table 87: Wyckoff bond: 4c@4m

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

Table 88: Wyckoff bond: 8d@4m

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

Table 89: Wyckoff bond: `8e@4m`

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

Table 90: Wyckoff bond: `8f@4m`

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

Table 91: Wyckoff bond: `16g@4m`

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

* Wyckoff site: 4n, site symmetry: m2m.

Table 92: Wyckoff bond: 4a@4n

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 93: Wyckoff bond: 4b@4n

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 94: Wyckoff bond: 4c@4n

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 95: Wyckoff bond: 8d@4n

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 96: Wyckoff bond: **8e@4n**

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 97: Wyckoff bond: **8f@4n**

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 98: Wyckoff bond: **16g@4n**

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: 4o, site symmetry: m2m.

Table 99: Wyckoff bond: 4a@4o

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

Table 100: Wyckoff bond: 4b@4o

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

Table 101: Wyckoff bond: 4c@4o

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

Table 102: Wyckoff bond: 8d@4o

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

Table 103: Wyckoff bond: 8e@4o

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

Table 104: Wyckoff bond: 8f@4o

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

Table 105: Wyckoff bond: 16g@4o

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

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

Table 106: Wyckoff bond: 8a@8p

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]
7	$[Y, X, 0]$	$[y, x, 0]$	[7,16]
8	$[-Y, -X, 0]$	$[-y, -x, 0]$	[8,15]

Table 107: Wyckoff bond: 8b@8p

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 108: Wyckoff bond: 16c@8p

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]

continued ...

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Table 108

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

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

Table 109: Wyckoff bond: 8a@8q

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

Table 110: Wyckoff bond: 8b@8q

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

Table 111: Wyckoff bond: 16c@8q

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

Table 111

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

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

Table 112: Wyckoff bond: `8a@8r`

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 113: Wyckoff bond: `8b@8r`

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 114: Wyckoff bond: `16c@8r`

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]

continued ...

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Table 114

No.	vector	center	mapping
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: `8s`, site symmetry: `.m.`

Table 115: Wyckoff bond: `8a@8s`

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

Table 116: Wyckoff bond: `8b@8s`

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

Table 117: Wyckoff bond: `16c@8s`

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

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

Table 118: Wyckoff bond: `8a@8t`

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

Table 119: Wyckoff bond: `8b@8t`

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

Table 120: Wyckoff bond: `16c@8t`

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

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

Table 121: Wyckoff bond: `16a@16u`

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]