

SG No. 47 D_{2h}^1 $Pmmm$ [orthorhombic]

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

* Wyckoff site: **1a**, site symmetry: **mmm**

Table 1: Wyckoff bond: **1a@1a**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	$[1, 2, -3, -4, -5, -6, 7, 8]$

Table 2: Wyckoff bond: **1b@1a**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, 0, 0]$	$[1, -2, 3, -4, -5, 6, -7, 8]$

Table 3: Wyckoff bond: **1c@1a**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, 0]$	$[1, -2, -3, 4, -5, 6, 7, -8]$

Table 4: Wyckoff bond: **2d@1a**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[0, 0, 0]$	$[3, -4, -7, 8]$

Table 5: Wyckoff bond: **2e@1a**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, 0]$	$[1, -3, -5, 7]$
2	$[-X, 0, Z]$	$[0, 0, 0]$	$[2, -4, -6, 8]$

Table 6: Wyckoff bond: **2f@1a**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, 0, 0]$	$[1, -4, -5, 8]$
2	$[0, -Y, Z]$	$[0, 0, 0]$	$[2, -3, -6, 7]$

Table 7: Wyckoff bond: **4g@1a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[0, 0, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, 0, 0]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[0, 0, 0]$	$[4, -8]$

* Wyckoff site: **1b**, site symmetry: **mmm**

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, 0]$	$[1, 2, -3, -4, -5, -6, 7, 8]$

Table 9: Wyckoff bond: **1b@1b**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, 0, 0]$	$[1, -2, 3, -4, -5, 6, -7, 8]$

Table 10: Wyckoff bond: **1c@1b**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, 0, 0]$	$[1, -2, -3, 4, -5, 6, 7, -8]$

Table 11: Wyckoff bond: **2d@1b**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, 0]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[\frac{1}{2}, 0, 0]$	$[3, -4, -7, 8]$

Table 12: Wyckoff bond: **2e@1b**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, 0, 0]$	$[1, -3, -5, 7]$
2	$[-X, 0, Z]$	$[\frac{1}{2}, 0, 0]$	$[2, -4, -6, 8]$

Table 13: Wyckoff bond: **2f@1b**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, 0, 0]$	$[1, -4, -5, 8]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, 0, 0]$	$[2, -3, -6, 7]$

Table 14: Wyckoff bond: **4g@1b**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, 0]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, 0]$	$[4, -8]$

* Wyckoff site: **1c**, site symmetry: **mmm**

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, \frac{1}{2}]$	$[1, 2, -3, -4, -5, -6, 7, 8]$

Table 16: Wyckoff bond: **1b@1c**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, 0, \frac{1}{2}]$	$[1, -2, 3, -4, -5, 6, -7, 8]$

Table 17: Wyckoff bond: **1c@1c**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, \frac{1}{2}]$	$[1, -2, -3, 4, -5, 6, 7, -8]$

Table 18: Wyckoff bond: **2d@1c**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, \frac{1}{2}]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[0, 0, \frac{1}{2}]$	$[3, -4, -7, 8]$

Table 19: Wyckoff bond: **2e@1c**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -3, -5, 7]$
2	$[-X, 0, Z]$	$[0, 0, \frac{1}{2}]$	$[2, -4, -6, 8]$

Table 20: Wyckoff bond: **2f@1c**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -4, -5, 8]$
2	$[0, -Y, Z]$	$[0, 0, \frac{1}{2}]$	$[2, -3, -6, 7]$

Table 21: Wyckoff bond: **4g@1c**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[0, 0, \frac{1}{2}]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, 0, \frac{1}{2}]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[0, 0, \frac{1}{2}]$	$[4, -8]$

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

Table 22: Wyckoff bond: **1a@1d**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, 2, -3, -4, -5, -6, 7, 8]$

Table 23: Wyckoff bond: **1b@1d**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, -2, 3, -4, -5, 6, -7, 8]$

Table 24: Wyckoff bond: **1c@1d**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, -2, -3, 4, -5, 6, 7, -8]$

Table 25: Wyckoff bond: 2d@1d

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[3, -4, -7, 8]$

Table 26: Wyckoff bond: 2e@1d

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, -3, -5, 7]$
2	$[-X, 0, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, -4, -6, 8]$

Table 27: Wyckoff bond: 2f@1d

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, -4, -5, 8]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, -3, -6, 7]$

Table 28: Wyckoff bond: 4g@1d

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[4, -8]$

* Wyckoff site: 1e, site symmetry: mmm

Table 29: Wyckoff bond: 1a@1e

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, 0]$	$[1, 2, -3, -4, -5, -6, 7, 8]$

Table 30: Wyckoff bond: 1b@1e

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, \frac{1}{2}, 0]$	$[1, -2, 3, -4, -5, 6, -7, 8]$

Table 31: Wyckoff bond: **1c@1e**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, \frac{1}{2}, 0]$	$[1, -2, -3, 4, -5, 6, 7, -8]$

Table 32: Wyckoff bond: **2d@1e**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, 0]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, 0]$	$[3, -4, -7, 8]$

Table 33: Wyckoff bond: **2e@1e**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, \frac{1}{2}, 0]$	$[1, -3, -5, 7]$
2	$[-X, 0, Z]$	$[0, \frac{1}{2}, 0]$	$[2, -4, -6, 8]$

Table 34: Wyckoff bond: **2f@1e**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, \frac{1}{2}, 0]$	$[1, -4, -5, 8]$
2	$[0, -Y, Z]$	$[0, \frac{1}{2}, 0]$	$[2, -3, -6, 7]$

Table 35: Wyckoff bond: **4g@1e**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, 0]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, 0]$	$[4, -8]$

* Wyckoff site: **1f**, site symmetry: **mmm**

Table 36: Wyckoff bond: **1a@1f**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, 2, -3, -4, -5, -6, 7, 8]$

Table 37: Wyckoff bond: **1b@1f**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, -2, 3, -4, -5, 6, -7, 8]$

Table 38: Wyckoff bond: **1c@1f**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, -2, -3, 4, -5, 6, 7, -8]$

Table 39: Wyckoff bond: **2d@1f**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[3, -4, -7, 8]$

Table 40: Wyckoff bond: **2e@1f**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, -3, -5, 7]$
2	$[-X, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, -4, -6, 8]$

Table 41: Wyckoff bond: **2f@1f**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, -4, -5, 8]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, -3, -6, 7]$

Table 42: Wyckoff bond: **4g@1f**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[4, -8]$

* Wyckoff site: **1g**, site symmetry: **mmm**

Table 43: Wyckoff bond: **1a@1g**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, -3, -4, -5, -6, 7, 8]$

Table 44: Wyckoff bond: **1b@1g**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, 3, -4, -5, 6, -7, 8]$

Table 45: Wyckoff bond: **1c@1g**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -3, 4, -5, 6, 7, -8]$

Table 46: Wyckoff bond: **2d@1g**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -4, -7, 8]$

Table 47: Wyckoff bond: **2e@1g**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -3, -5, 7]$
2	$[-X, 0, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -4, -6, 8]$

Table 48: Wyckoff bond: **2f@1g**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -4, -5, 8]$
2	$[0, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -3, -6, 7]$

Table 49: Wyckoff bond: **4g@1g**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[4, -8]$

* Wyckoff site: **1h**, site symmetry: **mmm**

Table 50: Wyckoff bond: **1a@1h**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, -3, -4, -5, -6, 7, 8]$

Table 51: Wyckoff bond: **1b@1h**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, 3, -4, -5, 6, -7, 8]$

Table 52: Wyckoff bond: **1c@1h**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -3, 4, -5, 6, 7, -8]$

Table 53: Wyckoff bond: **2d@1h**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -2, -5, 6]$
2	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3, -4, -7, 8]$

Table 54: Wyckoff bond: **2e@1h**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -3, -5, 7]$
2	$[-X, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, -4, -6, 8]$

Table 55: Wyckoff bond: 2f@1h

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -4, -5, 8]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, -3, -6, 7]$

Table 56: Wyckoff bond: 4g@1h

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

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

Table 57: Wyckoff bond: 2a@2i

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, 0, 0]$	$[1, -4, -6, 7]$
2	$[0, 0, Z]$	$[-x, 0, 0]$	$[2, -3, -5, 8]$

Table 58: Wyckoff bond: 2b@2i

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, 0, 0]$	$[1, -4, 6, -7]$
2	$[0, -Y, 0]$	$[-x, 0, 0]$	$[2, -3, 5, -8]$

Table 59: Wyckoff bond: 2c@2i

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	$[1, 4, 6, 7]$
2	$[-X, 0, 0]$	$[-x, 0, 0]$	$[2, 3, 5, 8]$

Table 60: Wyckoff bond: **4d@2i**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, 0, 0]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[-x, 0, 0]$	$[2, 5]$
3	$[-X, Y, 0]$	$[-x, 0, 0]$	$[3, 8]$
4	$[X, -Y, 0]$	$[x, 0, 0]$	$[4, 7]$

Table 61: Wyckoff bond: **4e@2i**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, 0]$	$[1, 7]$
2	$[-X, 0, Z]$	$[-x, 0, 0]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[-x, 0, 0]$	$[3, 5]$
4	$[X, 0, -Z]$	$[x, 0, 0]$	$[4, 6]$

Table 62: Wyckoff bond: **4f@2i**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[x, 0, 0]$	$[1, -4]$
2	$[0, -Y, Z]$	$[-x, 0, 0]$	$[2, -3]$
3	$[0, -Y, -Z]$	$[-x, 0, 0]$	$[5, -8]$
4	$[0, Y, -Z]$	$[x, 0, 0]$	$[6, -7]$

Table 63: Wyckoff bond: **8g@2i**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, 0, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, 0, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[x, 0, 0]$	$[4]$
5	$[-X, -Y, -Z]$	$[-x, 0, 0]$	$[5]$
6	$[X, Y, -Z]$	$[x, 0, 0]$	$[6]$
7	$[X, -Y, Z]$	$[x, 0, 0]$	$[7]$
8	$[-X, Y, Z]$	$[-x, 0, 0]$	$[8]$

* Wyckoff site: **2j**, site symmetry: **2mm**

Table 64: Wyckoff bond: 2a@2j

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, 0, \frac{1}{2}]$	$[1, -4, -6, 7]$
2	$[0, 0, Z]$	$[-x, 0, \frac{1}{2}]$	$[2, -3, -5, 8]$

Table 65: Wyckoff bond: 2b@2j

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, 0, \frac{1}{2}]$	$[1, -4, 6, -7]$
2	$[0, -Y, 0]$	$[-x, 0, \frac{1}{2}]$	$[2, -3, 5, -8]$

Table 66: Wyckoff bond: 2c@2j

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, \frac{1}{2}]$	$[1, 4, 6, 7]$
2	$[-X, 0, 0]$	$[-x, 0, \frac{1}{2}]$	$[2, 3, 5, 8]$

Table 67: Wyckoff bond: 4d@2j

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, 0, \frac{1}{2}]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[-x, 0, \frac{1}{2}]$	$[2, 5]$
3	$[-X, Y, 0]$	$[-x, 0, \frac{1}{2}]$	$[3, 8]$
4	$[X, -Y, 0]$	$[x, 0, \frac{1}{2}]$	$[4, 7]$

Table 68: Wyckoff bond: 4e@2j

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, \frac{1}{2}]$	$[1, 7]$
2	$[-X, 0, Z]$	$[-x, 0, \frac{1}{2}]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[-x, 0, \frac{1}{2}]$	$[3, 5]$
4	$[X, 0, -Z]$	$[x, 0, \frac{1}{2}]$	$[4, 6]$

Table 69: Wyckoff bond: **4f@2j**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[x, 0, \frac{1}{2}]$	$[1, -4]$
2	$[0, -Y, Z]$	$[-x, 0, \frac{1}{2}]$	$[2, -3]$
3	$[0, -Y, -Z]$	$[-x, 0, \frac{1}{2}]$	$[5, -8]$
4	$[0, Y, -Z]$	$[x, 0, \frac{1}{2}]$	$[6, -7]$

Table 70: Wyckoff bond: **8g@2j**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, \frac{1}{2}]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, 0, \frac{1}{2}]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, 0, \frac{1}{2}]$	$[3]$
4	$[X, -Y, -Z]$	$[x, 0, \frac{1}{2}]$	$[4]$
5	$[-X, -Y, -Z]$	$[-x, 0, \frac{1}{2}]$	$[5]$
6	$[X, Y, -Z]$	$[x, 0, \frac{1}{2}]$	$[6]$
7	$[X, -Y, Z]$	$[x, 0, \frac{1}{2}]$	$[7]$
8	$[-X, Y, Z]$	$[-x, 0, \frac{1}{2}]$	$[8]$

* Wyckoff site: **2k**, site symmetry: **2mm**

Table 71: Wyckoff bond: **2a@2k**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, \frac{1}{2}, 0]$	$[1, -4, -6, 7]$
2	$[0, 0, Z]$	$[-x, \frac{1}{2}, 0]$	$[2, -3, -5, 8]$

Table 72: Wyckoff bond: **2b@2k**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, \frac{1}{2}, 0]$	$[1, -4, 6, -7]$
2	$[0, -Y, 0]$	$[-x, \frac{1}{2}, 0]$	$[2, -3, 5, -8]$

Table 73: Wyckoff bond: **2c@2k**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, \frac{1}{2}, 0]$	$[1, 4, 6, 7]$
2	$[-X, 0, 0]$	$[-x, \frac{1}{2}, 0]$	$[2, 3, 5, 8]$

Table 74: Wyckoff bond: **4d@2k**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, \frac{1}{2}, 0]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[-x, \frac{1}{2}, 0]$	$[2, 5]$
3	$[-X, Y, 0]$	$[-x, \frac{1}{2}, 0]$	$[3, 8]$
4	$[X, -Y, 0]$	$[x, \frac{1}{2}, 0]$	$[4, 7]$

Table 75: Wyckoff bond: **4e@2k**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, \frac{1}{2}, 0]$	$[1, 7]$
2	$[-X, 0, Z]$	$[-x, \frac{1}{2}, 0]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[-x, \frac{1}{2}, 0]$	$[3, 5]$
4	$[X, 0, -Z]$	$[x, \frac{1}{2}, 0]$	$[4, 6]$

Table 76: Wyckoff bond: **4f@2k**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[x, \frac{1}{2}, 0]$	$[1, -4]$
2	$[0, -Y, Z]$	$[-x, \frac{1}{2}, 0]$	$[2, -3]$
3	$[0, -Y, -Z]$	$[-x, \frac{1}{2}, 0]$	$[5, -8]$
4	$[0, Y, -Z]$	$[x, \frac{1}{2}, 0]$	$[6, -7]$

Table 77: Wyckoff bond: **8g@2k**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, \frac{1}{2}, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, \frac{1}{2}, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, \frac{1}{2}, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[x, \frac{1}{2}, 0]$	$[4]$
5	$[-X, -Y, -Z]$	$[-x, \frac{1}{2}, 0]$	$[5]$
6	$[X, Y, -Z]$	$[x, \frac{1}{2}, 0]$	$[6]$
7	$[X, -Y, Z]$	$[x, \frac{1}{2}, 0]$	$[7]$
8	$[-X, Y, Z]$	$[-x, \frac{1}{2}, 0]$	$[8]$

* Wyckoff site: 21, site symmetry: $2mm$

Table 78: Wyckoff bond: 2a@21

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, -4, -6, 7]$
2	$[0, 0, Z]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, -3, -5, 8]$

Table 79: Wyckoff bond: 2b@21

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, -4, 6, -7]$
2	$[0, -Y, 0]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, -3, 5, -8]$

Table 80: Wyckoff bond: 2c@21

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, 4, 6, 7]$
2	$[-X, 0, 0]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, 3, 5, 8]$

Table 81: Wyckoff bond: 4d@21

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, 5]$
3	$[-X, Y, 0]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[3, 8]$
4	$[X, -Y, 0]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[4, 7]$

Table 82: Wyckoff bond: 4e@21

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, 7]$
2	$[-X, 0, Z]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[3, 5]$
4	$[X, 0, -Z]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[4, 6]$

Table 83: Wyckoff bond: **4f@21**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[1, -4]$
2	$[0, -Y, Z]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[2, -3]$
3	$[0, -Y, -Z]$	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[5, -8]$
4	$[0, Y, -Z]$	$[x, \frac{1}{2}, \frac{1}{2}]$	$[6, -7]$

Table 84: Wyckoff bond: **8g@21**

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

* Wyckoff site: **2m**, site symmetry: **m2m**

Table 85: Wyckoff bond: **2a@2m**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, y, 0]$	$[1, -3, -6, 8]$
2	$[0, 0, Z]$	$[0, -y, 0]$	$[2, -4, -5, 7]$

Table 86: Wyckoff bond: **2b@2m**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, y, 0]$	$[1, 3, 6, 8]$
2	$[0, -Y, 0]$	$[0, -y, 0]$	$[2, 4, 5, 7]$

Table 87: Wyckoff bond: **2c@2m**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, 0]$	$[1, -3, 6, -8]$
2	$[-X, 0, 0]$	$[0, -y, 0]$	$[2, -4, 5, -7]$

Table 88: Wyckoff bond: **4d@2m**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, y, 0]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[0, -y, 0]$	$[2, 5]$
3	$[-X, Y, 0]$	$[0, y, 0]$	$[3, 8]$
4	$[X, -Y, 0]$	$[0, -y, 0]$	$[4, 7]$

Table 89: Wyckoff bond: **4e@2m**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, y, 0]$	$[1, -3]$
2	$[-X, 0, Z]$	$[0, -y, 0]$	$[2, -4]$
3	$[-X, 0, -Z]$	$[0, -y, 0]$	$[5, -7]$
4	$[X, 0, -Z]$	$[0, y, 0]$	$[6, -8]$

Table 90: Wyckoff bond: **4f@2m**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, 0]$	$[1, 8]$
2	$[0, -Y, Z]$	$[0, -y, 0]$	$[2, 7]$
3	$[0, Y, -Z]$	$[0, y, 0]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[0, -y, 0]$	$[4, 5]$

Table 91: Wyckoff bond: **8g@2m**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[0, -y, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[0, y, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[0, -y, 0]$	$[4]$
5	$[-X, -Y, -Z]$	$[0, -y, 0]$	$[5]$
6	$[X, Y, -Z]$	$[0, y, 0]$	$[6]$
7	$[X, -Y, Z]$	$[0, -y, 0]$	$[7]$
8	$[-X, Y, Z]$	$[0, y, 0]$	$[8]$

* Wyckoff site: **2n**, site symmetry: **m2m**

Table 92: Wyckoff bond: 2a@2n

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, y, \frac{1}{2}]$	$[1, -3, -6, 8]$
2	$[0, 0, Z]$	$[0, -y, \frac{1}{2}]$	$[2, -4, -5, 7]$

Table 93: Wyckoff bond: 2b@2n

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, y, \frac{1}{2}]$	$[1, 3, 6, 8]$
2	$[0, -Y, 0]$	$[0, -y, \frac{1}{2}]$	$[2, 4, 5, 7]$

Table 94: Wyckoff bond: 2c@2n

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, \frac{1}{2}]$	$[1, -3, 6, -8]$
2	$[-X, 0, 0]$	$[0, -y, \frac{1}{2}]$	$[2, -4, 5, -7]$

Table 95: Wyckoff bond: 4d@2n

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, y, \frac{1}{2}]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[0, -y, \frac{1}{2}]$	$[2, 5]$
3	$[-X, Y, 0]$	$[0, y, \frac{1}{2}]$	$[3, 8]$
4	$[X, -Y, 0]$	$[0, -y, \frac{1}{2}]$	$[4, 7]$

Table 96: Wyckoff bond: 4e@2n

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, y, \frac{1}{2}]$	$[1, -3]$
2	$[-X, 0, Z]$	$[0, -y, \frac{1}{2}]$	$[2, -4]$
3	$[-X, 0, -Z]$	$[0, -y, \frac{1}{2}]$	$[5, -7]$
4	$[X, 0, -Z]$	$[0, y, \frac{1}{2}]$	$[6, -8]$

Table 97: Wyckoff bond: **4f@2n**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, \frac{1}{2}]$	$[1, 8]$
2	$[0, -Y, Z]$	$[0, -y, \frac{1}{2}]$	$[2, 7]$
3	$[0, Y, -Z]$	$[0, y, \frac{1}{2}]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[0, -y, \frac{1}{2}]$	$[4, 5]$

Table 98: Wyckoff bond: **8g@2n**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, \frac{1}{2}]$	$[1]$
2	$[-X, -Y, Z]$	$[0, -y, \frac{1}{2}]$	$[2]$
3	$[-X, Y, -Z]$	$[0, y, \frac{1}{2}]$	$[3]$
4	$[X, -Y, -Z]$	$[0, -y, \frac{1}{2}]$	$[4]$
5	$[-X, -Y, -Z]$	$[0, -y, \frac{1}{2}]$	$[5]$
6	$[X, Y, -Z]$	$[0, y, \frac{1}{2}]$	$[6]$
7	$[X, -Y, Z]$	$[0, -y, \frac{1}{2}]$	$[7]$
8	$[-X, Y, Z]$	$[0, y, \frac{1}{2}]$	$[8]$

* Wyckoff site: **2o**, site symmetry: **m2m**

Table 99: Wyckoff bond: **2a@2o**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, y, 0]$	$[1, -3, -6, 8]$
2	$[0, 0, Z]$	$[\frac{1}{2}, -y, 0]$	$[2, -4, -5, 7]$

Table 100: Wyckoff bond: **2b@2o**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, y, 0]$	$[1, 3, 6, 8]$
2	$[0, -Y, 0]$	$[\frac{1}{2}, -y, 0]$	$[2, 4, 5, 7]$

Table 101: Wyckoff bond: **2c@2o**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, y, 0]$	$[1, -3, 6, -8]$
2	$[-X, 0, 0]$	$[\frac{1}{2}, -y, 0]$	$[2, -4, 5, -7]$

Table 102: Wyckoff bond: **4d@2o**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, y, 0]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[\frac{1}{2}, -y, 0]$	$[2, 5]$
3	$[-X, Y, 0]$	$[\frac{1}{2}, y, 0]$	$[3, 8]$
4	$[X, -Y, 0]$	$[\frac{1}{2}, -y, 0]$	$[4, 7]$

Table 103: Wyckoff bond: **4e@2o**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, y, 0]$	$[1, -3]$
2	$[-X, 0, Z]$	$[\frac{1}{2}, -y, 0]$	$[2, -4]$
3	$[-X, 0, -Z]$	$[\frac{1}{2}, -y, 0]$	$[5, -7]$
4	$[X, 0, -Z]$	$[\frac{1}{2}, y, 0]$	$[6, -8]$

Table 104: Wyckoff bond: **4f@2o**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, y, 0]$	$[1, 8]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, -y, 0]$	$[2, 7]$
3	$[0, Y, -Z]$	$[\frac{1}{2}, y, 0]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[\frac{1}{2}, -y, 0]$	$[4, 5]$

Table 105: Wyckoff bond: **8g@2o**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, y, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, -y, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[\frac{1}{2}, y, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, -y, 0]$	$[4]$
5	$[-X, -Y, -Z]$	$[\frac{1}{2}, -y, 0]$	$[5]$
6	$[X, Y, -Z]$	$[\frac{1}{2}, y, 0]$	$[6]$
7	$[X, -Y, Z]$	$[\frac{1}{2}, -y, 0]$	$[7]$
8	$[-X, Y, Z]$	$[\frac{1}{2}, y, 0]$	$[8]$

* Wyckoff site: **2p**, site symmetry: **m2m**

Table 106: Wyckoff bond: **2a@2p**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[1, -3, -6, 8]$
2	$[0, 0, Z]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[2, -4, -5, 7]$

Table 107: Wyckoff bond: **2b@2p**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[1, 3, 6, 8]$
2	$[0, -Y, 0]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[2, 4, 5, 7]$

Table 108: Wyckoff bond: **2c@2p**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[1, -3, 6, -8]$
2	$[-X, 0, 0]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[2, -4, 5, -7]$

Table 109: Wyckoff bond: **4d@2p**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[2, 5]$
3	$[-X, Y, 0]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[3, 8]$
4	$[X, -Y, 0]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[4, 7]$

Table 110: Wyckoff bond: **4e@2p**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[1, -3]$
2	$[-X, 0, Z]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[2, -4]$
3	$[-X, 0, -Z]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[5, -7]$
4	$[X, 0, -Z]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[6, -8]$

Table 111: Wyckoff bond: **4f02p**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[1, 8]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[2, 7]$
3	$[0, Y, -Z]$	$[\frac{1}{2}, y, \frac{1}{2}]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[\frac{1}{2}, -y, \frac{1}{2}]$	$[4, 5]$

Table 112: Wyckoff bond: **8g02p**

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

* Wyckoff site: **2q**, site symmetry: **mm2**

Table 113: Wyckoff bond: **2a02q**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	$[1, 2, 7, 8]$
2	$[0, 0, -Z]$	$[0, 0, -z]$	$[3, 4, 5, 6]$

Table 114: Wyckoff bond: **2b02q**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, 0, z]$	$[1, -2, -7, 8]$
2	$[0, Y, 0]$	$[0, 0, -z]$	$[3, -4, -5, 6]$

Table 115: Wyckoff bond: **2c02q**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, z]$	$[1, -2, 7, -8]$
2	$[-X, 0, 0]$	$[0, 0, -z]$	$[3, -4, 5, -6]$

Table 116: Wyckoff bond: **4d@2q**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, 0, -z]$	$[3, -4]$
3	$[-X, -Y, 0]$	$[0, 0, -z]$	$[5, -6]$
4	$[X, -Y, 0]$	$[0, 0, z]$	$[7, -8]$

Table 117: Wyckoff bond: **4e@2q**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, z]$	$[1, 7]$
2	$[-X, 0, Z]$	$[0, 0, z]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[0, 0, -z]$	$[3, 5]$
4	$[X, 0, -Z]$	$[0, 0, -z]$	$[4, 6]$

Table 118: Wyckoff bond: **4f@2q**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, 0, z]$	$[1, 8]$
2	$[0, -Y, Z]$	$[0, 0, z]$	$[2, 7]$
3	$[0, Y, -Z]$	$[0, 0, -z]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[0, 0, -z]$	$[4, 5]$

Table 119: Wyckoff bond: **8g@2q**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	$[1]$
2	$[-X, -Y, Z]$	$[0, 0, z]$	$[2]$
3	$[-X, Y, -Z]$	$[0, 0, -z]$	$[3]$
4	$[X, -Y, -Z]$	$[0, 0, -z]$	$[4]$
5	$[-X, -Y, -Z]$	$[0, 0, -z]$	$[5]$
6	$[X, Y, -Z]$	$[0, 0, -z]$	$[6]$
7	$[X, -Y, Z]$	$[0, 0, z]$	$[7]$
8	$[-X, Y, Z]$	$[0, 0, z]$	$[8]$

* Wyckoff site: **2r**, site symmetry: **mm2**

Table 120: Wyckoff bond: **2a@2r**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, \frac{1}{2}, z]$	$[1, 2, 7, 8]$
2	$[0, 0, -Z]$	$[0, \frac{1}{2}, -z]$	$[3, 4, 5, 6]$

Table 121: Wyckoff bond: **2b@2r**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, \frac{1}{2}, z]$	$[1, -2, -7, 8]$
2	$[0, Y, 0]$	$[0, \frac{1}{2}, -z]$	$[3, -4, -5, 6]$

Table 122: Wyckoff bond: **2c@2r**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, \frac{1}{2}, z]$	$[1, -2, 7, -8]$
2	$[-X, 0, 0]$	$[0, \frac{1}{2}, -z]$	$[3, -4, 5, -6]$

Table 123: Wyckoff bond: **4d@2r**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, \frac{1}{2}, z]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, \frac{1}{2}, -z]$	$[3, -4]$
3	$[-X, -Y, 0]$	$[0, \frac{1}{2}, -z]$	$[5, -6]$
4	$[X, -Y, 0]$	$[0, \frac{1}{2}, z]$	$[7, -8]$

Table 124: Wyckoff bond: **4e@2r**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, \frac{1}{2}, z]$	$[1, 7]$
2	$[-X, 0, Z]$	$[0, \frac{1}{2}, z]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[0, \frac{1}{2}, -z]$	$[3, 5]$
4	$[X, 0, -Z]$	$[0, \frac{1}{2}, -z]$	$[4, 6]$

Table 125: Wyckoff bond: **4f@2r**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, \frac{1}{2}, z]$	$[1, 8]$
2	$[0, -Y, Z]$	$[0, \frac{1}{2}, z]$	$[2, 7]$
3	$[0, Y, -Z]$	$[0, \frac{1}{2}, -z]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[0, \frac{1}{2}, -z]$	$[4, 5]$

Table 126: Wyckoff bond: **8g@2r**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, \frac{1}{2}, z]$	$[1]$
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, z]$	$[2]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, -z]$	$[3]$
4	$[X, -Y, -Z]$	$[0, \frac{1}{2}, -z]$	$[4]$
5	$[-X, -Y, -Z]$	$[0, \frac{1}{2}, -z]$	$[5]$
6	$[X, Y, -Z]$	$[0, \frac{1}{2}, -z]$	$[6]$
7	$[X, -Y, Z]$	$[0, \frac{1}{2}, z]$	$[7]$
8	$[-X, Y, Z]$	$[0, \frac{1}{2}, z]$	$[8]$

* Wyckoff site: **2s**, site symmetry: **mm2**

Table 127: Wyckoff bond: **2a@2s**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, 0, z]$	$[1, 2, 7, 8]$
2	$[0, 0, -Z]$	$[\frac{1}{2}, 0, -z]$	$[3, 4, 5, 6]$

Table 128: Wyckoff bond: **2b@2s**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, 0, z]$	$[1, -2, -7, 8]$
2	$[0, Y, 0]$	$[\frac{1}{2}, 0, -z]$	$[3, -4, -5, 6]$

Table 129: Wyckoff bond: **2c@2s**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, 0, z]$	$[1, -2, 7, -8]$
2	$[-X, 0, 0]$	$[\frac{1}{2}, 0, -z]$	$[3, -4, 5, -6]$

Table 130: Wyckoff bond: **4d@2s**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, 0, z]$	$[1, -2]$
2	$[-X, Y, 0]$	$[\frac{1}{2}, 0, -z]$	$[3, -4]$
3	$[-X, -Y, 0]$	$[\frac{1}{2}, 0, -z]$	$[5, -6]$
4	$[X, -Y, 0]$	$[\frac{1}{2}, 0, z]$	$[7, -8]$

Table 131: Wyckoff bond: **4e@2s**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, 0, z]$	$[1, 7]$
2	$[-X, 0, Z]$	$[\frac{1}{2}, 0, z]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[\frac{1}{2}, 0, -z]$	$[3, 5]$
4	$[X, 0, -Z]$	$[\frac{1}{2}, 0, -z]$	$[4, 6]$

Table 132: Wyckoff bond: **4f@2s**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, 0, z]$	$[1, 8]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, 0, z]$	$[2, 7]$
3	$[0, Y, -Z]$	$[\frac{1}{2}, 0, -z]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[\frac{1}{2}, 0, -z]$	$[4, 5]$

Table 133: Wyckoff bond: **8g@2s**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, z]$	$[1]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, z]$	$[2]$
3	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, -z]$	$[3]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, -z]$	$[4]$
5	$[-X, -Y, -Z]$	$[\frac{1}{2}, 0, -z]$	$[5]$
6	$[X, Y, -Z]$	$[\frac{1}{2}, 0, -z]$	$[6]$
7	$[X, -Y, Z]$	$[\frac{1}{2}, 0, z]$	$[7]$
8	$[-X, Y, Z]$	$[\frac{1}{2}, 0, z]$	$[8]$

* Wyckoff site: **2t**, site symmetry: **mm2**

Table 134: Wyckoff bond: **2a@2t**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 2, 7, 8]$
2	$[0, 0, -Z]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[3, 4, 5, 6]$

Table 135: Wyckoff bond: **2b@2t**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, -2, -7, 8]$
2	$[0, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[3, -4, -5, 6]$

Table 136: Wyckoff bond: **2c@2t**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, -2, 7, -8]$
2	$[-X, 0, 0]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[3, -4, 5, -6]$

Table 137: Wyckoff bond: **4d@2t**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, -2]$
2	$[-X, Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[3, -4]$
3	$[-X, -Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[5, -6]$
4	$[X, -Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[7, -8]$

Table 138: Wyckoff bond: **4e@2t**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 7]$
2	$[-X, 0, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[3, 5]$
4	$[X, 0, -Z]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[4, 6]$

Table 139: Wyckoff bond: **4f@2t**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[1, 8]$
2	$[0, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[2, 7]$
3	$[0, Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[4, 5]$

Table 140: Wyckoff bond: **8g@2t**

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

* Wyckoff site: **4u**, site symmetry: **m**.

Table 141: Wyckoff bond: **4a@4u**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, y, z]$	$[1, 8]$
2	$[0, -Y, Z]$	$[0, -y, z]$	$[2, 7]$
3	$[0, Y, -Z]$	$[0, y, -z]$	$[3, 6]$
4	$[0, -Y, -Z]$	$[0, -y, -z]$	$[4, 5]$

Table 142: Wyckoff bond: **4b@4u**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, y, z]$	$[1, -8]$
2	$[-X, 0, 0]$	$[0, -y, z]$	$[2, -7]$
3	$[-X, 0, 0]$	$[0, y, -z]$	$[3, -6]$
4	$[X, 0, 0]$	$[0, -y, -z]$	$[4, -5]$

Table 143: Wyckoff bond: **8c@4u**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, z]$	[1]
2	$[-X, -Y, Z]$	$[0, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[0, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[0, -y, -z]$	[4]
5	$[-X, -Y, -Z]$	$[0, -y, -z]$	[5]
6	$[X, Y, -Z]$	$[0, y, -z]$	[6]
7	$[X, -Y, Z]$	$[0, -y, z]$	[7]
8	$[-X, Y, Z]$	$[0, y, z]$	[8]

* Wyckoff site: **4v**, site symmetry: **m**..

Table 144: Wyckoff bond: **4a@4v**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[\frac{1}{2}, y, z]$	[1, 8]
2	$[0, -Y, Z]$	$[\frac{1}{2}, -y, z]$	[2, 7]
3	$[0, Y, -Z]$	$[\frac{1}{2}, y, -z]$	[3, 6]
4	$[0, -Y, -Z]$	$[\frac{1}{2}, -y, -z]$	[4, 5]

Table 145: Wyckoff bond: **4b@4v**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[\frac{1}{2}, y, z]$	[1, -8]
2	$[-X, 0, 0]$	$[\frac{1}{2}, -y, z]$	[2, -7]
3	$[-X, 0, 0]$	$[\frac{1}{2}, y, -z]$	[3, -6]
4	$[X, 0, 0]$	$[\frac{1}{2}, -y, -z]$	[4, -5]

Table 146: Wyckoff bond: **8c@4v**

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

* Wyckoff site: **4w**, site symmetry: **.m**.

Table 147: Wyckoff bond: **4a@4w**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, 0, z]$	$[1, 7]$
2	$[-X, 0, Z]$	$[-x, 0, z]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[-x, 0, -z]$	$[3, 5]$
4	$[X, 0, -Z]$	$[x, 0, -z]$	$[4, 6]$

Table 148: Wyckoff bond: **4b@4w**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, 0, z]$	$[1, -7]$
2	$[0, -Y, 0]$	$[-x, 0, z]$	$[2, -8]$
3	$[0, Y, 0]$	$[-x, 0, -z]$	$[3, -5]$
4	$[0, -Y, 0]$	$[x, 0, -z]$	$[4, -6]$

Table 149: Wyckoff bond: **8c@4w**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, z]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, 0, z]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, 0, -z]$	$[3]$
4	$[X, -Y, -Z]$	$[x, 0, -z]$	$[4]$
5	$[-X, -Y, -Z]$	$[-x, 0, -z]$	$[5]$
6	$[X, Y, -Z]$	$[x, 0, -z]$	$[6]$
7	$[X, -Y, Z]$	$[x, 0, z]$	$[7]$
8	$[-X, Y, Z]$	$[-x, 0, z]$	$[8]$

* Wyckoff site: **4x**, site symmetry: **.m**.

Table 150: Wyckoff bond: **4a@4x**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[x, \frac{1}{2}, z]$	$[1, 7]$
2	$[-X, 0, Z]$	$[-x, \frac{1}{2}, z]$	$[2, 8]$
3	$[-X, 0, -Z]$	$[-x, \frac{1}{2}, -z]$	$[3, 5]$
4	$[X, 0, -Z]$	$[x, \frac{1}{2}, -z]$	$[4, 6]$

Table 151: Wyckoff bond: **4b@4x**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[x, \frac{1}{2}, z]$	$[1, -7]$
2	$[0, -Y, 0]$	$[-x, \frac{1}{2}, z]$	$[2, -8]$
3	$[0, Y, 0]$	$[-x, \frac{1}{2}, -z]$	$[3, -5]$
4	$[0, -Y, 0]$	$[x, \frac{1}{2}, -z]$	$[4, -6]$

Table 152: Wyckoff bond: **8c@4x**

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	$[-X, Y, -Z]$	$[-x, \frac{1}{2}, -z]$	$[3]$
4	$[X, -Y, -Z]$	$[x, \frac{1}{2}, -z]$	$[4]$
5	$[-X, -Y, -Z]$	$[-x, \frac{1}{2}, -z]$	$[5]$
6	$[X, Y, -Z]$	$[x, \frac{1}{2}, -z]$	$[6]$
7	$[X, -Y, Z]$	$[x, \frac{1}{2}, z]$	$[7]$
8	$[-X, Y, Z]$	$[-x, \frac{1}{2}, z]$	$[8]$

* Wyckoff site: **4y**, site symmetry: $\bar{3}m$

Table 153: Wyckoff bond: **4a@4y**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, y, 0]$	$[1, 6]$
2	$[-X, -Y, 0]$	$[-x, -y, 0]$	$[2, 5]$
3	$[-X, Y, 0]$	$[-x, y, 0]$	$[3, 8]$
4	$[X, -Y, 0]$	$[x, -y, 0]$	$[4, 7]$

Table 154: Wyckoff bond: **4b@4y**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, y, 0]$	$[1, -6]$
2	$[0, 0, Z]$	$[-x, -y, 0]$	$[2, -5]$
3	$[0, 0, -Z]$	$[-x, y, 0]$	$[3, -8]$
4	$[0, 0, -Z]$	$[x, -y, 0]$	$[4, -7]$

Table 155: Wyckoff bond: **8c@4y**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, 0]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, 0]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, 0]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, 0]$	[4]
5	$[-X, -Y, -Z]$	$[-x, -y, 0]$	[5]
6	$[X, Y, -Z]$	$[x, y, 0]$	[6]
7	$[X, -Y, Z]$	$[x, -y, 0]$	[7]
8	$[-X, Y, Z]$	$[-x, y, 0]$	[8]

* Wyckoff site: **4z**, site symmetry: $\bar{4}2m$

Table 156: Wyckoff bond: **4a@4z**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, y, \frac{1}{2}]$	[1,6]
2	$[-X, -Y, 0]$	$[-x, -y, \frac{1}{2}]$	[2,5]
3	$[-X, Y, 0]$	$[-x, y, \frac{1}{2}]$	[3,8]
4	$[X, -Y, 0]$	$[x, -y, \frac{1}{2}]$	[4,7]

Table 157: Wyckoff bond: **4b@4z**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, y, \frac{1}{2}]$	[1,-6]
2	$[0, 0, Z]$	$[-x, -y, \frac{1}{2}]$	[2,-5]
3	$[0, 0, -Z]$	$[-x, y, \frac{1}{2}]$	[3,-8]
4	$[0, 0, -Z]$	$[x, -y, \frac{1}{2}]$	[4,-7]

Table 158: Wyckoff bond: **8c@4z**

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

* Wyckoff site: **8A**, site symmetry: **1**

Table 159: Wyckoff bond: **8a@8A**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, -Y, Z]$	$[-x, -y, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, y, -z]$	[3]
4	$[X, -Y, -Z]$	$[x, -y, -z]$	[4]
5	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[5]
6	$[X, Y, -Z]$	$[x, y, -z]$	[6]
7	$[X, -Y, Z]$	$[x, -y, z]$	[7]
8	$[-X, Y, Z]$	$[-x, y, z]$	[8]