

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: 4f@2p

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: 8g@2p

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: 2a@2q

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: 2b@2q

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: 2c@2q

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: ...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: . . m

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]