

SG No. 71  $D_{2h}^{25}$   $Immm$  [ orthorhombic ]

\* plus set:  $+ [0, 0, 0], + [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

\* Wyckoff site: **2a**, site symmetry: **mmm**

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

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

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

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

Table 3: Wyckoff bond: **2c@2a**

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

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

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: **4e@2a**

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: **4f@2a**

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: **8g@2a**

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: **2b**, site symmetry: **mmm**

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

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

Table 9: Wyckoff bond: **2b@2b**

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

Table 10: Wyckoff bond: **2c@2b**

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

Table 11: Wyckoff bond: **4d@2b**

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 12: Wyckoff bond: **4e@2b**

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 13: Wyckoff bond: 4f@2b

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 14: Wyckoff bond: 8g@2b

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: 2c, site symmetry: mmm

Table 15: Wyckoff bond: 2a@2c

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

Table 16: Wyckoff bond: 2b@2c

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

Table 17: Wyckoff bond: 2c@2c

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

Table 18: Wyckoff bond: 4d@2c

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 19: Wyckoff bond: **4e@2c**

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 20: Wyckoff bond: **4f@2c**

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 21: Wyckoff bond: **8g@2c**

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: **2d**, site symmetry: **mmm**

Table 22: Wyckoff bond: **2a@2d**

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: **2b@2d**

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: **2c@2d**

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: 4d@2d

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: 4e@2d

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: 4f@2d

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: 8g@2d

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: 4e, site symmetry: 2mm

Table 29: Wyckoff bond: 4a@4e

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 30: Wyckoff bond: **4b@4e**

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 31: Wyckoff bond: **4c@4e**

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 32: Wyckoff bond: **8d@4e**

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 33: Wyckoff bond: **8e@4e**

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 34: Wyckoff bond: **8f@4e**

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 35: Wyckoff bond: **16g@4e**

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: **4f**, site symmetry: **2mm**

Table 36: Wyckoff bond: **4a@4f**

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 37: Wyckoff bond: **4b@4f**

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 38: Wyckoff bond: **4c@4f**

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 39: Wyckoff bond: **8d@4f**

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 40: Wyckoff bond: **8e@4f**

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 41: Wyckoff bond: **8f@4f**

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 42: Wyckoff bond: **16g@4f**

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: **4g**, site symmetry: **m2m**

Table 43: Wyckoff bond: **4a@4g**

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

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, y, 0]$	$[1, 3, 6, 8]$

*continued ...*



Table 44

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

Table 45: Wyckoff bond:  $4c@4g$ 

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 46: Wyckoff bond:  $8d@4g$ 

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 47: Wyckoff bond:  $8e@4g$ 

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 48: Wyckoff bond:  $8f@4g$ 

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 49: Wyckoff bond: **16g@4g**

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: **4h**, site symmetry: **m2m**

Table 50: Wyckoff bond: **4a@4h**

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

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

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 53: Wyckoff bond: **8d@4h**

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 54: Wyckoff bond: **8e@4h**

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 55: Wyckoff bond: **8f@4h**

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 56: Wyckoff bond: **16g@4h**

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: **4i**, site symmetry: **mm2**

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

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

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

*continued ...*

Table 58

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

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

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

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

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 62: Wyckoff bond:  $8f@4i$ 

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

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: **4j**, site symmetry: **mm2**

Table 64: Wyckoff bond: **4a@4j**

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 65: Wyckoff bond: **4b@4j**

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 66: Wyckoff bond: **4c@4j**

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 67: Wyckoff bond: **8d@4j**

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

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

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

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: **8k**, site symmetry:  $-1$

Table 71: Wyckoff bond: **8a@8k**

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

\* Wyckoff site: **8l**, site symmetry:  $m..$

Table 72: Wyckoff bond: **8a@81**

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 73: Wyckoff bond: **8b@81**

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 74: Wyckoff bond: **16c@81**

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

Table 75: Wyckoff bond: **8a@8m**

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 76: Wyckoff bond: **8b@8m**

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 77: Wyckoff bond: **16c@8m**

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: **8n**, site symmetry:  $\bar{3}m$

Table 78: Wyckoff bond: **8a@8n**

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 79: Wyckoff bond: **8b@8n**

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 80: Wyckoff bond: **16c@8n**

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: **16o**, site symmetry: 1

Table 81: Wyckoff bond: **16a@16o**

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]