

SG No. 177 D_6^1 $P622$ [hexagonal]

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

* Wyckoff site: **1a**, site symmetry: **622**

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

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

Table 2: Wyckoff bond: **3b@1a**

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

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

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

Table 4: Wyckoff bond: **6d@1a**

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

Table 5: Wyckoff bond: **6e@1a**

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[0, 0, 0]$	$[1, -8]$
2	$[-2X, -X, Z]$	$[0, 0, 0]$	$[2, -7]$
3	$[X, -X, Z]$	$[0, 0, 0]$	$[3, -9]$

continued ...

Table 5

No.	vector	center	mapping
4	$[-X, -2X, Z]$	$[0, 0, 0]$	$[4, -11]$
5	$[2X, X, Z]$	$[0, 0, 0]$	$[5, -10]$
6	$[-X, X, Z]$	$[0, 0, 0]$	$[6, -12]$

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

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

Table 7: Wyckoff bond: **12g@1a**

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

* Wyckoff site: **1b**, site symmetry: **622**

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

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

Table 9: Wyckoff bond: **3b@1b**

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

Table 10: Wyckoff bond: **3c@1b**

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

Table 11: Wyckoff bond: **6d@1b**

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

Table 12: Wyckoff bond: **6e@1b**

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

Table 13: Wyckoff bond: **6f@1b**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -11]$
2	$[0, X, Z]$	$[0, 0, \frac{1}{2}]$	$[2, -10]$

continued ...

Table 13

No.	vector	center	mapping
3	$[-X, -X, Z]$	$[0, 0, \frac{1}{2}]$	[3,-12]
4	$[-X, 0, Z]$	$[0, 0, \frac{1}{2}]$	[4,-8]
5	$[0, -X, Z]$	$[0, 0, \frac{1}{2}]$	[5,-7]
6	$[X, X, Z]$	$[0, 0, \frac{1}{2}]$	[6,-9]

Table 14: Wyckoff bond: **12g@1b**

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

* Wyckoff site: **2c**, site symmetry: **3.2**

Table 15: Wyckoff bond: **2a@2c**

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

Table 16: Wyckoff bond: **6b@2c**

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

Table 17: Wyckoff bond: 6c@2c

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

Table 18: Wyckoff bond: 12d@2c

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

* Wyckoff site: 2d, site symmetry: 3.2

Table 19: Wyckoff bond: 2a@2d

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

Table 20: Wyckoff bond: 6b@2d

No.	vector	center	mapping
1	$[X, 0, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[1, -11]$
2	$[0, X, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[2, -10]$
3	$[-X, -X, Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[3, -12]$
4	$[-X, 0, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[4, -8]$
5	$[0, -X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[5, -7]$

continued ...

Table 20

No.	vector	center	mapping
6	$[X, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[6, -9]$

Table 21: Wyckoff bond: 6c@2d

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

Table 22: Wyckoff bond: 12d@2d

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

* Wyckoff site: 2e, site symmetry: 6..

Table 23: Wyckoff bond: 2a@2e

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

Table 24: Wyckoff bond: **6b@2e**

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

Table 25: Wyckoff bond: **12c@2e**

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

* Wyckoff site: **3f**, site symmetry: **222**

Table 26: Wyckoff bond: **3a@3f**

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

Table 27: Wyckoff bond: **3b@3f**

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

Table 28: Wyckoff bond: **3c@3f**

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

Table 29: Wyckoff bond: **6d@3f**

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

Table 30: Wyckoff bond: **6e@3f**

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

Table 31: Wyckoff bond: **6f@3f**

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

Table 32: Wyckoff bond: 12g@3f

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

* Wyckoff site: 3g, site symmetry: 222

Table 33: Wyckoff bond: 3a@3g

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

Table 34: Wyckoff bond: 3b@3g

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

Table 35: Wyckoff bond: 3c@3g

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

Table 36: Wyckoff bond: **6d@3g**

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

Table 37: Wyckoff bond: **6e@3g**

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

Table 38: Wyckoff bond: **6f@3g**

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

Table 39: Wyckoff bond: **12g@3g**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[1]$
2	$[-Y, X - Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[2]$
3	$[-X + Y, -X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[3]$
4	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[4]$
5	$[Y, -X + Y, Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[5]$
6	$[X - Y, X, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[6]$
7	$[Y, X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[7]$
8	$[X - Y, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[8]$
9	$[-X, -X + Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[9]$

continued ...

Table 39

No.	vector	center	mapping
10	$[-Y, -X, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[12]

* Wyckoff site: 4h, site symmetry: 3..

Table 40: Wyckoff bond: 4a@4h

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

Table 41: Wyckoff bond: 12b@4h

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

* Wyckoff site: 6i, site symmetry: 2..

Table 42: Wyckoff bond: 6a@6i

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

Table 43: Wyckoff bond: **6b@6i**

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

Table 44: Wyckoff bond: **12c@6i**

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

* Wyckoff site: **6j**, site symmetry: $.2.$

Table 45: Wyckoff bond: **6a@6j**

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

Table 46: Wyckoff bond: **6b@6j**

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

Table 47: Wyckoff bond: **12c@6j**

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

* Wyckoff site: **6k**, site symmetry: $.2$.

Table 48: Wyckoff bond: **6a@6k**

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

Table 49: Wyckoff bond: **6b@6k**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, \frac{1}{2}]$	$[1, 8]$

continued ...

Table 49

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

Table 50: Wyckoff bond: **12c@6k**

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

* Wyckoff site: **6l**, site symmetry: $\dots 2$

Table 51: Wyckoff bond: **6a@6l**

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

Table 52: Wyckoff bond: **6b@6l**

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, -x, 0]$	$[1, 10]$
2	$[X, 2X, 0]$	$[x, 2x, 0]$	$[2, 12]$
3	$[-2X, -X, 0]$	$[-2x, -x, 0]$	$[3, 11]$

continued ...

Table 52

No.	vector	center	mapping
4	$[-X, X, 0]$	$[-x, x, 0]$	$[4, 7]$
5	$[-X, -2X, 0]$	$[-x, -2x, 0]$	$[5, 9]$
6	$[2X, X, 0]$	$[2x, x, 0]$	$[6, 8]$

Table 53: Wyckoff bond: **12c@61**

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

* Wyckoff site: **6m**, site symmetry: $\bar{3}2$

Table 54: Wyckoff bond: **6a@6m**

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

Table 55: Wyckoff bond: **6b@6m**

No.	vector	center	mapping
1	$[X, -X, 0]$	$[x, -x, \frac{1}{2}]$	$[1, 10]$
2	$[X, 2X, 0]$	$[x, 2x, \frac{1}{2}]$	$[2, 12]$
3	$[-2X, -X, 0]$	$[-2x, -x, \frac{1}{2}]$	$[3, 11]$
4	$[-X, X, 0]$	$[-x, x, \frac{1}{2}]$	$[4, 7]$
5	$[-X, -2X, 0]$	$[-x, -2x, \frac{1}{2}]$	$[5, 9]$

continued ...

Table 55

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

Table 56: Wyckoff bond: 12c@6m

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

* Wyckoff site: 12n, site symmetry: 1

Table 57: Wyckoff bond: 12a@12n

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