

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: 61, site symmetry: . . 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: ...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]