

SG No. 182  $D_6^6$   $P6_322$  [ hexagonal ]

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

\* Wyckoff site: **2a**, site symmetry: **32**.

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

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

Table 2: Wyckoff bond: **6b@2a**

No.	vector	center	mapping
1	$[X, 2X, Z]$	$[0, 0, 0]$	$[1, -8]$
2	$[-2X, -X, Z]$	$[0, 0, 0]$	$[2, -7]$
3	$[X, -X, Z]$	$[0, 0, 0]$	$[3, -9]$
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 3: Wyckoff bond: **6c@2a**

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

Table 4: Wyckoff bond: **12d@2a**

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	$[-X, -Y, Z]$	$[0, 0, \frac{1}{2}]$	$[4]$
5	$[Y, -X + Y, Z]$	$[0, 0, \frac{1}{2}]$	$[5]$
6	$[X - Y, X, Z]$	$[0, 0, \frac{1}{2}]$	$[6]$
7	$[Y, X, -Z]$	$[0, 0, 0]$	$[7]$
8	$[X - Y, -Y, -Z]$	$[0, 0, 0]$	$[8]$
9	$[-X, -X + Y, -Z]$	$[0, 0, 0]$	$[9]$

*continued ...*

Table 4

No.	vector	center	mapping
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: 2b, site symmetry: 3.2

Table 5: Wyckoff bond: 2a@2b

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

Table 6: Wyckoff bond: 6b@2b

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

Table 7: Wyckoff bond: 6c@2b

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

Table 8: Wyckoff bond: 12d@2b

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

*continued ...*

Table 8

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

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

Table 9: Wyckoff bond: 2a@2c

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

Table 10: Wyckoff bond: 6b@2c

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

Table 11: Wyckoff bond: 6c@2c

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

Table 12: Wyckoff bond: 12d@2c

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

\* Wyckoff site: 2d, site symmetry: 3.2

Table 13: Wyckoff bond: 2a@2d

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

Table 14: Wyckoff bond: 6b@2d

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

Table 15: Wyckoff bond: 6c@2d

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

continued ...

Table 15

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

Table 16: Wyckoff bond: 12d@2d

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

\* Wyckoff site: 4e, site symmetry: 3..

Table 17: Wyckoff bond: 4a@4e

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

Table 18: Wyckoff bond: 12b@4e

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	$[-X, -Y, Z]$	$[0, 0, z + \frac{1}{2}]$	[4]
5	$[Y, -X + Y, Z]$	$[0, 0, z + \frac{1}{2}]$	[5]
6	$[X - Y, X, Z]$	$[0, 0, z + \frac{1}{2}]$	[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]

*continued ...*

Table 18

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

\* Wyckoff site: 4f, site symmetry:  $3..$

Table 19: Wyckoff bond: 4a@4f

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

Table 20: Wyckoff bond: 12b@4f

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	$[-X, -Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[4]
5	$[Y, -X + Y, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[5]
6	$[X - Y, X, Z]$	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[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	$[-Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[10]
11	$[-X + Y, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[11]
12	$[X, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[12]

\* Wyckoff site: 6g, site symmetry:  $.2.$

Table 21: Wyckoff bond: 6a@6g

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	$[-X, -2X, Z]$	$[-x, 0, \frac{1}{2}]$	[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 22: Wyckoff bond:  $6b@6g$ 

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	$[-X, 0, 0]$	$[-x, 0, \frac{1}{2}]$	$[4, 11]$
5	$[0, -X, 0]$	$[0, -x, \frac{1}{2}]$	$[5, 10]$
6	$[X, X, 0]$	$[x, x, \frac{1}{2}]$	$[6, 12]$

Table 23: Wyckoff bond:  $12c@6g$ 

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	$[-X, -Y, Z]$	$[-x, 0, \frac{1}{2}]$	$[4]$
5	$[Y, -X + Y, Z]$	$[0, -x, \frac{1}{2}]$	$[5]$
6	$[X - Y, X, Z]$	$[x, x, \frac{1}{2}]$	$[6]$
7	$[Y, X, -Z]$	$[0, x, 0]$	$[7]$
8	$[X - Y, -Y, -Z]$	$[x, 0, 0]$	$[8]$
9	$[-X, -X + Y, -Z]$	$[-x, -x, 0]$	$[9]$
10	$[-Y, -X, -Z]$	$[0, -x, \frac{1}{2}]$	$[10]$
11	$[-X + Y, Y, -Z]$	$[-x, 0, \frac{1}{2}]$	$[11]$
12	$[X, X - Y, -Z]$	$[x, x, \frac{1}{2}]$	$[12]$

\* Wyckoff site:  $6h$ , site symmetry:  $. . 2$

Table 24: Wyckoff bond:  $6a@6h$ 

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

Table 25: Wyckoff bond: 6b@6h

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

Table 26: Wyckoff bond: 12c@6h

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

\* Wyckoff site: 12i, site symmetry: 1

Table 27: Wyckoff bond: 12a@12i

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	$[-X, -Y, Z]$	$[-x, -y, z + \frac{1}{2}]$	[4]
5	$[Y, -X + Y, Z]$	$[y, -x + y, z + \frac{1}{2}]$	[5]
6	$[X - Y, X, Z]$	$[x - y, x, z + \frac{1}{2}]$	[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	$[-Y, -X, -Z]$	$[-y, -x, \frac{1}{2} - z]$	[10]
11	$[-X + Y, Y, -Z]$	$[-x + y, y, \frac{1}{2} - z]$	[11]
12	$[X, X - Y, -Z]$	$[x, x - y, \frac{1}{2} - z]$	[12]