

SG No. 174  $C_{3h}^1 P\bar{6}$  [ hexagonal ]

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

\* Wyckoff site: **1a**, site symmetry:  $-6..$

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

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

Table 2: Wyckoff bond: **3b@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	$[-X + Y, -X, 0]$	$[0, 0, 0]$	$[3, 6]$

Table 3: Wyckoff bond: **6c@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	$[-X + Y, -X, -Z]$	$[0, 0, 0]$	$[6]$

\* Wyckoff site: **1b**, site symmetry:  $-6..$

Table 4: Wyckoff bond: **1a@1b**

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

Table 5: Wyckoff bond: **3b@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	$[-X + Y, -X, 0]$	$[0, 0, \frac{1}{2}]$	$[3, 6]$

Table 6: Wyckoff bond: **6c@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]

\* Wyckoff site: 1c, site symmetry:  $-6..$

Table 7: Wyckoff bond: **1a@1c**

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

Table 8: Wyckoff bond: **3b@1c**

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

Table 9: Wyckoff bond: **6c@1c**

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	$[X, Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	[4]
5	$[-Y, X - Y, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	[5]
6	$[-X + Y, -X, -Z]$	$[\frac{1}{3}, \frac{2}{3}, 0]$	[6]

\* Wyckoff site: 1d, site symmetry:  $-6..$

Table 10: Wyckoff bond: **1a@1d**

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

Table 11: Wyckoff bond: **3b@1d**

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

Table 12: Wyckoff bond: **6c@1d**

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

\* Wyckoff site: **1e**, site symmetry:  $-6..$

Table 13: Wyckoff bond: **1a@1e**

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

Table 14: Wyckoff bond: **3b@1e**

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

Table 15: Wyckoff bond: **6c@1e**

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

\* Wyckoff site: 1f, site symmetry:  $-6..$

Table 16: Wyckoff bond: **1a@1f**

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

Table 17: Wyckoff bond: **3b@1f**

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

Table 18: Wyckoff bond: **6c@1f**

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

\* Wyckoff site: 2g, site symmetry:  $3..$

Table 19: Wyckoff bond: **2a@2g**

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

Table 20: Wyckoff bond: **6b@2g**

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	$[-Y, X - Y, -Z]$	$[0, 0, -z]$	$[5]$

*continued ...*

Table 20

No.	vector	center	mapping
6	$[-X + Y, -X, -Z]$	$[0, 0, -z]$	[6]

\* Wyckoff site: 2h, site symmetry:  $3..$

Table 21: Wyckoff bond: 2a@2h

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

Table 22: Wyckoff bond: 6b@2h

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

\* Wyckoff site: 2i, site symmetry:  $3..$

Table 23: Wyckoff bond: 2a@2i

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

Table 24: Wyckoff bond: 6b@2i

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

\* Wyckoff site: 3j, site symmetry:  $m..$

Table 25: Wyckoff bond: 3a@3j

No.	vector	center	mapping
1	$[X, Y, 0]$	$[x, y, 0]$	$[1, 4]$
2	$[-Y, X - Y, 0]$	$[-y, x - y, 0]$	$[2, 5]$
3	$[-X + Y, -X, 0]$	$[-x + y, -x, 0]$	$[3, 6]$

Table 26: Wyckoff bond: 3b@3j

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, y, 0]$	$[1, -4]$
2	$[0, 0, Z]$	$[-y, x - y, 0]$	$[2, -5]$
3	$[0, 0, Z]$	$[-x + y, -x, 0]$	$[3, -6]$

Table 27: Wyckoff bond: 6c@3j

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, 0]$	$[1]$
2	$[-Y, X - Y, Z]$	$[-y, x - y, 0]$	$[2]$
3	$[-X + Y, -X, Z]$	$[-x + y, -x, 0]$	$[3]$
4	$[X, Y, -Z]$	$[x, y, 0]$	$[4]$
5	$[-Y, X - Y, -Z]$	$[-y, x - y, 0]$	$[5]$
6	$[-X + Y, -X, -Z]$	$[-x + y, -x, 0]$	$[6]$

\* Wyckoff site: 3k, site symmetry:  $m..$

Table 28: Wyckoff bond: 3a@3k

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

Table 29: Wyckoff bond: 3b@3k

No.	vector	center	mapping
1	$[0, 0, Z]$	$[x, y, \frac{1}{2}]$	$[1, -4]$
2	$[0, 0, Z]$	$[-y, x - y, \frac{1}{2}]$	$[2, -5]$

*continued ...*

Table 29

No.	vector	center	mapping
3	$[0, 0, Z]$	$[-x + y, -x, \frac{1}{2}]$	[3, -6]

Table 30: Wyckoff bond: 6c@3k

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

\* Wyckoff site: 6l, site symmetry: 1

Table 31: Wyckoff bond: 6a@6l

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]