

SG No. 168 C_6^1 $P6$ [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, z]	[1,2,3,4,5,6]

Table 2: Wyckoff bond: 3b@1a

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]

Table 3: Wyckoff bond: 6c@1a

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]

* Wyckoff site: 2b, site symmetry: 3..

Table 4: Wyckoff bond: 2a@2b

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]

Table 5: Wyckoff bond: 6b@2b

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]

continued ...

Table 5

No.	vector	center	mapping
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: 3c, site symmetry: 2..

Table 6: Wyckoff bond: 3a@3c

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]

Table 7: Wyckoff bond: 3b@3c

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]

Table 8: Wyckoff bond: 6c@3c

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]

* Wyckoff site: 6d, site symmetry: 1

Table 9: Wyckoff bond: 6a@6d

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]

continued ...

Table 9

No.	vector	center	mapping
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]