

SG No. 172 $C_6^5 P6_4$ [hexagonal]

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

* Wyckoff site: **3a**, site symmetry: $2..$

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

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

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

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

Table 3: Wyckoff bond: **6c@3a**

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

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

Table 4: Wyckoff bond: **3a@3b**

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

Table 5: Wyckoff bond: **3b@3b**

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

Table 6: Wyckoff bond: **6c@3b**

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

* Wyckoff site: **6c**, site symmetry: **1**

Table 7: Wyckoff bond: **6a@6c**

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