

PG No. 21 C_6 6 [hexagonal]

* 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: **6b**, site symmetry: 1

Table 4: Wyckoff bond: **6a@6b**

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	$[X - Y, X, Z]$	$[x - y, x, z]$	$[6]$