

MSG No. 168.109 $P6$ [Type I, hexagonal]

Table 1: Wyckoff site: **1a**, site symmetry: 6..

No.	position	mapping
1	[0, 0, z]	[1,2,3,4,5,6]

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

No.	position	mapping
1	$\left[\frac{1}{3}, \frac{2}{3}, z\right]$	[1,3,5]
2	$\left[\frac{2}{3}, \frac{1}{3}, z\right]$	[2,4,6]

Table 3: Wyckoff site: **3c**, site symmetry: 2..

No.	position	mapping
1	$\left[\frac{1}{2}, 0, z\right]$	[1,4]
2	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[2,5]
3	$\left[0, \frac{1}{2}, z\right]$	[3,6]

Table 4: Wyckoff site: **6d**, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[x - y, x, z]	[2]
3	[-y, x - y, z]	[3]
4	[-x, -y, z]	[4]
5	[-x + y, -x, z]	[5]
6	[y, -x + y, z]	[6]