

MSG No. 168.111 $P6'$ [Type III, 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	[$\frac{1}{3}$, $\frac{2}{3}$, z]	[1,2,3]
2	[$\frac{2}{3}$, $\frac{1}{3}$, z]	[4,5,6]

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

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

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

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