

MSG No. 173.130 $P6_31'$ [Type II, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: 3..1'

No.	position	mapping
1	[0, 0, z]	[1,3,5,7,9,11]
2	[0, 0, $z + \frac{1}{2}$]	[2,4,6,8,10,12]

Table 2: Wyckoff site: 2b, site symmetry: 3..1'

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	[1,3,5,7,9,11]
2	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[2,4,6,8,10,12]

Table 3: Wyckoff site: 6c, site symmetry: 11'

No.	position	mapping
1	[x, y, z]	[1,7]
2	$[x - y, x, z + \frac{1}{2}]$	[2,8]
3	$[-y, x - y, z]$	[3,9]
4	$[-x, -y, z + \frac{1}{2}]$	[4,10]
5	$[-x + y, -x, z]$	[5,11]
6	$[y, -x + y, z + \frac{1}{2}]$	[6,12]