

MSG No. 186.203 $P6_3mc$ [Type I, hexagonal]

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

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

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

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

Table 3: Wyckoff site: 6c, site symmetry: .m.

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

Table 4: Wyckoff site: 12d, site symmetry: 1

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