

MSG No. 168.112 P_c6 [Type IV, hexagonal]

Table 1: Wyckoff site: 2a, site symmetry: 6..

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

Table 2: Wyckoff site: 4b, site symmetry: 3..

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

Table 3: Wyckoff site: 6c, site symmetry: 2..

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

Table 4: Wyckoff site: 12d, 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]
7	$[x, y, z + \frac{1}{2}]$	[7]
8	$[x - y, x, z + \frac{1}{2}]$	[8]
9	$[-y, x - y, z + \frac{1}{2}]$	[9]
10	$[-x, -y, z + \frac{1}{2}]$	[10]
11	$[-x + y, -x, z + \frac{1}{2}]$	[11]
12	$[y, -x + y, z + \frac{1}{2}]$	[12]