

MSG No. 157.56 P_c31m [Type IV, trigonal]

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

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	$[\frac{1}{3}, \frac{2}{3}, z]$	[1,2,3]
2	$[\frac{2}{3}, \frac{1}{3}, z]$	[4,5,6]
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	[7,8,9]
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[10,11,12]

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

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

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

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