

MSG No. 159.63  $P31c'$  [ Type III, trigonal ]

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

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

Table 3: Wyckoff site: 6c, 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 + $\frac{1}{2}$ ]	[4]
5	[x - y, -y, z + $\frac{1}{2}$ ]	[5]
6	[y, x, z + $\frac{1}{2}$ ]	[6]