

MSG No. 152.33 $P3_121$ [Type I, trigonal]

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

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

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

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

Table 3: Wyckoff site: **6c**, site symmetry: 1

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