

MSG No. 157.53  $P31m$  [ Type I, trigonal ]

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6]$

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

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

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

No.	position	mapping
1	$[x, 0, z]$	$[1, 5]$
2	$[0, x, z]$	$[2, 6]$
3	$[-x, -x, z]$	$[3, 4]$

Table 4: Wyckoff site: 6d, 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	$[y, x, z]$	$[6]$