

MSG No. 157.54 $P31m1'$ [Type II, trigonal]

Table 1: Wyckoff site: $1a$, site symmetry: $3.m1'$

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

Table 2: Wyckoff site: $2b$, site symmetry: $3..1'$

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

Table 3: Wyckoff site: $3c$, site symmetry: $..m1'$

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

Table 4: Wyckoff site: $6d$, site symmetry: $11'$

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