

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: 3b, site symmetry:  $.m$

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

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	$[y, x, z]$	$[4]$
5	$[x - y, -y, z]$	$[5]$
6	$[-x, -x + y, z]$	$[6]$