

Table 1: Wyckoff site: **1a**, site symmetry: $6..$

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

Table 2: Wyckoff site: **6b**, site symmetry: 1

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