

Table 1: Wyckoff site: $1o$, site symmetry: $\bar{3}1'$

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

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

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

Table 3: Wyckoff site: $6b$, site symmetry: 1

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