

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: -6

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

Table 2: Wyckoff site: $2\mathbf{a}$, site symmetry: $3.$

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

Table 3: Wyckoff site: $3\mathbf{b}$, site symmetry: $\mathbf{m}.$

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

Table 4: Wyckoff site: $6\mathbf{c}$, site symmetry: 1

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