

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

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: 3b, site symmetry: $m..$

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

Table 4: Wyckoff site: 6c, 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	$[x, y, -z]$	$[5, 11]$
5	$[-y, x - y, -z]$	$[6, 12]$
6	$[-x + y, -x, -z]$	$[4, 10]$