

Table 1: Wyckoff site: 1o, site symmetry: $6/m'$

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: $6..$

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

Table 3: Wyckoff site: 6b, site symmetry: $m'..$

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

Table 4: Wyckoff site: 12c, 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	$[x - y, x, z]$	$[2]$
7	$[-x, -y, -z]$	$[7]$
8	$[y, -x + y, -z]$	$[9]$
9	$[x - y, x, -z]$	$[11]$
10	$[x, y, -z]$	$[10]$
11	$[-y, x - y, -z]$	$[12]$
12	$[-x + y, -x, -z]$	$[8]$