

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $6'/\mathbf{m}'$

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

Table 2: Wyckoff site: $2\mathbf{a}$, site symmetry: $6'..$

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: $6\mathbf{b}$, site symmetry: $\mathbf{m}'..$

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

Table 4: Wyckoff site: $12\mathbf{c}$, site symmetry: 1

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