

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $4/m$

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

Table 2: Wyckoff site: $2\mathbf{a}$, site symmetry: $4..$

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

Table 3: Wyckoff site: $4\mathbf{b}$, site symmetry: $m..$

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

Table 4: Wyckoff site: $8\mathbf{c}$, site symmetry: 1

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