

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $4/m1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]$

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 9, 10, 11, 12]$
2	$[0, 0, -z]$	$[5, 6, 7, 8, 13, 14, 15, 16]$

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

No.	position	mapping
1	$[x, y, 0]$	$[1, 6, 9, 14]$
2	$[-x, -y, 0]$	$[2, 5, 10, 13]$
3	$[-y, x, 0]$	$[3, 8, 11, 16]$
4	$[y, -x, 0]$	$[4, 7, 12, 15]$

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

No.	position	mapping
1	$[x, y, z]$	$[1, 9]$
2	$[-x, -y, z]$	$[2, 10]$
3	$[-y, x, z]$	$[3, 11]$
4	$[y, -x, z]$	$[4, 12]$
5	$[-x, -y, -z]$	$[5, 13]$
6	$[x, y, -z]$	$[6, 14]$
7	$[y, -x, -z]$	$[7, 15]$
8	$[-y, x, -z]$	$[8, 16]$