

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $2'2'2$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4]$

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 3]$
2	$[-x, 0, 0]$	$[2, 4]$

Table 3: Wyckoff site: $2\mathbf{b}$, site symmetry: $.2'.$

No.	position	mapping
1	$[0, y, 0]$	$[1, 4]$
2	$[0, -y, 0]$	$[2, 3]$

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2]$
2	$[0, 0, -z]$	$[3, 4]$

Table 5: Wyckoff site: $4\mathbf{d}$, site symmetry: 1

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