

Table 1: Wyckoff site:  $1\mathbf{o}$ , site symmetry:  $23$ 

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

Table 2: Wyckoff site:  $4\mathbf{a}$ , site symmetry:  $.3.$ 

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

Table 3: Wyckoff site:  $6\mathbf{b}$ , site symmetry:  $2..$ 

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

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

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