

Table 1: Wyckoff site: **4a**, site symmetry:  $\cdot \cdot 2$

No.	position	mapping
1	$[x, x, 0]$	$[1, 3]$
2	$[-x, -x, \frac{1}{2}]$	$[2, 4]$
3	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	$[5, 8]$
4	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	$[6, 7]$

Table 2: Wyckoff site: **8b**, site symmetry:  $1$

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