

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

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

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

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