

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

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