

Table 1: Wyckoff site: 4a, site symmetry:  $.m'$ .

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

Table 2: Wyckoff site: 4b, site symmetry:  $.m'$ .

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

Table 3: Wyckoff site: 8c, site symmetry: 1

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