

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

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

Table 2: Wyckoff site: 4b, site symmetry:  $\dots 2'$

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

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

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