

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

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

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

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

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

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