

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $..2'$

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

Table 4: Wyckoff site: 8d, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[x, -y, \frac{1}{2} - z]$	[6]
7	$[\frac{1}{2} - x, y, -z]$	[7]
8	$[-x, \frac{1}{2} - y, z]$	[8]