

Table 1: Wyckoff site: 4a, site symmetry: $-1'$

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

Table 2: Wyckoff site: 4b, site symmetry: $-1'$

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

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

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

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	$[x, -y, z + \frac{1}{2}]$	[3]
4	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[4]
5	$[-x, y, \frac{1}{2} - z]$	[5]
6	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[6]
7	$[-x, -y, -z]$	[7]
8	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[8]