

Table 1: Wyckoff site: 8a, site symmetry: 2..

No.	position	mapping
1	$[0, 0, z]$	[1,2]
2	$[0, 0, z + \frac{1}{2}]$	[3,4]
3	$[0, \frac{1}{2}, z + \frac{1}{4}]$	[5,6]
4	$[\frac{1}{2}, 0, z + \frac{1}{4}]$	[7,8]
5	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9,10]
6	$[\frac{1}{2}, \frac{1}{2}, z]$	[11,12]
7	$[\frac{1}{2}, 0, z + \frac{3}{4}]$	[13,14]
8	$[0, \frac{1}{2}, z + \frac{3}{4}]$	[15,16]

Table 2: Wyckoff site: 16b, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[-x, y, z + \frac{1}{2}]$	[3]
4	$[x, -y, z + \frac{1}{2}]$	[4]
5	$[-y, x + \frac{1}{2}, z + \frac{1}{4}]$	[5]
6	$[y, \frac{1}{2} - x, z + \frac{1}{4}]$	[6]
7	$[\frac{1}{2} - y, -x, z + \frac{1}{4}]$	[7]
8	$[y + \frac{1}{2}, x, z + \frac{1}{4}]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]
10	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[10]
11	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[11]
12	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[12]
13	$[\frac{1}{2} - y, x, z + \frac{3}{4}]$	[13]
14	$[y + \frac{1}{2}, -x, z + \frac{3}{4}]$	[14]
15	$[-y, \frac{1}{2} - x, z + \frac{3}{4}]$	[15]
16	$[y, x + \frac{1}{2}, z + \frac{3}{4}]$	[16]