

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

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

Table 2: Wyckoff site: 8b, site symmetry:  $.m$ .

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

Table 3: Wyckoff site: 16c, site symmetry:  $1$

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