

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry:  $..m$ 

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

Table 4: Wyckoff site: 16d, site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x, z + \frac{1}{2}]$	[2]
3	$[y, -x, z + \frac{1}{2}]$	[3]
4	$[-x, -y, z]$	[4]
5	$[-x, y, z + \frac{1}{2}]$	[5]
6	$[x, -y, z + \frac{1}{2}]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]

*continued ...*

Table 4

No.	position	mapping
10	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[10]
11	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[11]
12	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[15]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[16]