

Table 1: Wyckoff site: 4a, site symmetry:  $m'm2'$ 

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

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

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

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

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

Table 4: Wyckoff site: 8d, site symmetry:  $.m.$ 

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

*continued ...*

Table 4

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

Table 5: Wyckoff site: **16e**, 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	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[6]
7	$[-x, y + \frac{1}{2}, z]$	[7]
8	$[x, \frac{1}{2} - y, z]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[9]
10	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[10]
11	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[11]
12	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[12]
13	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[14]
15	$[\frac{1}{2} - x, y, z]$	[15]
16	$[x + \frac{1}{2}, -y, z]$	[16]