

Table 1: Wyckoff site: 8a, site symmetry: $m..$

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

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

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

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

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

continued ...

Table 3

No.	position	mapping
16	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]