

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

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

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

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

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

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

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

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

continued ...

Table 4

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