

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

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

Table 2: Wyckoff site: 4b, site symmetry: 2.m'm'

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

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

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

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	$[-x, y, z + \frac{1}{2}]$	[5]
6	$[x, -y, z + \frac{1}{2}]$	[6]
7	$[-y, -x, z + \frac{1}{2}]$	[7]
8	$[y, x, z + \frac{1}{2}]$	[8]
9	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[9]

*continued ...*

Table 4

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