

MSG No. 108.236 $I4'cm'$ [Type III, tetragonal]

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

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

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

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

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

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