MSG No. 104.209 P_C4nc [Type IV, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: 2'..

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

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

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{2} - y,\ x + \frac{1}{2},\ z\right]$	[10]
11	$\left[y + \frac{1}{2},\ \frac{1}{2} - x,\ z\right]$	[11]
12	$\left[\frac{1}{2} - x,\ \frac{1}{2} - y,\ z\right]$	[12]
13	$\left[-x,\ y,\ z + \frac{1}{2}\right]$	[13]
14	$\left[x,\ -y,\ z + \frac{1}{2}\right]$	[14]
15	$\left[-y,\ -x,\ z + \frac{1}{2}\right]$	[15]
16	$\left[y,\ x,\ z + \frac{1}{2}\right]$	[16]

$\left[\frac{1}{2} - y,\ x + \frac{1}{2},\ z\right]$

$\left[y + \frac{1}{2},\ \frac{1}{2} - x,\ z\right]$

$\left[\frac{1}{2} - x,\ \frac{1}{2} - y,\ z\right]$

$\left[-x,\ y,\ z + \frac{1}{2}\right]$

2 $\frac{1}{2}$