MSG No. 99.169 P_C4mm [Type IV, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `4mm`

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

Table 2: Wyckoff site: `2b`, site symmetry: `4'mm'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2.mm`

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

Table 4: Wyckoff site: `8d`, site symmetry: `.m.`

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

Table 5: Wyckoff site: `8e`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,8]`
2	$[-x,\ x,\ z]$	`[2,5]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: ..m'

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

Table 7: Wyckoff site: 16g, 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	$[-x, y, z]$	[5]
6	$[x, -y, z]$	[6]
7	$[-y, -x, z]$	[7]
8	$[y, x, z]$	[8]
9	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z\right]$	[9]
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	$\left[\frac{1}{2}-x, y+\frac{1}{2}, z\right]$	[13]
14	$\left[x+\frac{1}{2}, \frac{1}{2}-y, z\right]$	[14]
15	$\left[\frac{1}{2}-y, \frac{1}{2}-x, z\right]$	[15]
16	$\left[y+\frac{1}{2}, x+\frac{1}{2}, z\right]$	[16]