MSG No. 99.168 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	$\left[0, 0, z+\frac{1}{2}\right]$	[9,10,11,12,13,14,15,16]

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, 0, z]$	[1,6]
2	$[0, x, z]$	[2,8]

continued ...

Table 5

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

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

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

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	$\left[x,\,y,\,z+\frac{1}{2}\right]$	[9]
10	$\left[-y,\,x,\,z+\frac{1}{2}\right]$	[10]
11	$\left[y,\,-x,\,z+\frac{1}{2}\right]$	[11]
12	$\left[-x,\,-y,\,z+\frac{1}{2}\right]$	[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]