MSG No. 107.230 $I4'mm'$ [Type III, tetragonal]

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

No.	position	mapping
1	$[0,\, 0,\, z]$	[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 2: Wyckoff site: 4b, site symmetry: 2mm.

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

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

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

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

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

Table 5: Wyckoff site: 16e, site symmetry: 1

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