MSG No. 98.159 $I4_1'22'$ [Type III, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 2.2'2'

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

Table 2: Wyckoff site: 4b, site symmetry: 2.2'2'

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: ..2'

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

Table 5: Wyckoff site: `8e`, site symmetry: `..2'`

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

Table 6: Wyckoff site: `8f`, site symmetry: `.2.`

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

Table 7: Wyckoff site: `16g`, site symmetry: `1`

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