MSG No. 98.161 $I4_1'2'2$ [Type III, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

Table 2: Wyckoff site: 4b, site symmetry: 2.22

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

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

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

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

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

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

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

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

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

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

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