MSG No. 41.216 A_aba2 [Type IV, orthorhombic]

Table 1: Wyckoff site: 8a, site symmetry: ..2

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

Table 2: Wyckoff site: 8b, site symmetry: ..2'

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

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

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

Table 4: Wyckoff site: 16d, site symmetry: 1

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