MSG No. 41.218 A_Bba2 [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `m'm'2`

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

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

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

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

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

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

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

continued ...

Table 4

No.	position	mapping
6	$\left[-x,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[6,11]
7	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ z\right]$	[7,10]
8	$\left[x+\frac{1}{2},\ \frac{1}{2},\ z\right]$	[8,9]

Table 5: Wyckoff site: 16e, 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	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[9]
10	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[10]
11	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[11]
12	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[12]
13	$\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[13]
14	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	[14]
15	$[-x,\ y,\ z]$	[15]
16	$[x,\ -y,\ z]$	[16]