MSG No. 39.201 A_bbm2 [Type IV, orthorhombic]

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

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

Table 2: Wyckoff site: `4b`, site symmetry: `m'm2'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `m'm'2`

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

Table 4: Wyckoff site: `4d`, site symmetry: `m'm2'`

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

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

No.	position	mapping
1	$[x,\ 0,\ z]$	`[1,12]`
2	$[-x,\ 0,\ z]$	`[2,11]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: .m.

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

Table 7: Wyckoff site: 8g, site symmetry: m'..

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

Table 8: Wyckoff site: 8h, site symmetry: m'..

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

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[6,16]
7	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[7,13]
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[8,14]

Table 9: Wyckoff site: 16i, site symmetry: 1

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