MSG No. 45.239 I_cba2 [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	$\left[\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[5,6,15,16]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ z\right]$	`[7,8,13,14]`

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

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

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

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

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

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

Table 5: Wyckoff site: `8e`, 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	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[5,15]`
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 6: Wyckoff site: `16f`, 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	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[5]`
6	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[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	$\left[x,\ y,\ z+\frac{1}{2}\right]$	`[9]`
10	$\left[-x,\ -y,\ z+\frac{1}{2}\right]$	`[10]`
11	$[-x,\ y,\ z]$	`[11]`
12	$[x,\ -y,\ z]$	`[12]`
13	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	`[13]`
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	`[14]`
15	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[15]`
16	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[16]`