MSG No. 61.440 P_Ibca [Type IV, orthorhombic]

Table 1: Wyckoff site: `8a`, site symmetry: `-1'`

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

Table 2: Wyckoff site: `8b`, site symmetry: `-1`

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

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

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

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

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

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

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

Table 6: Wyckoff site: `16f`, site symmetry: `1`

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