MSG No. 68.516 $Ccc'a'$ [Type III, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `22'2'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `22'2'`

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

Table 3: Wyckoff site: `8c`, site symmetry: `-1`

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

Table 4: Wyckoff site: `8d`, site symmetry: `-1`

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `.2'.`

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

Table 7: Wyckoff site: `8g`, site symmetry: `..2'`

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

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

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

continued ...

Table 8

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

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

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