MSG No. 68.517 $Cc'c'a'$ [Type III, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `222`

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

Table 2: Wyckoff site: `4b`, site symmetry: `222`

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ 0,\ z\right]$	`[1,12]`
2	$\left[\frac{1}{4},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[2,11]`
3	$\left[\frac{3}{4},\ 0,\ \frac{1}{2}-z\right]$	`[3,10]`

continued ...

Table 8

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

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	$\left[-x, y, \frac{1}{2}-z\right]$	[3]
4	$\left[-x, \frac{1}{2}-y, z\right]$	[4]
5	$\left[\frac{1}{2}-x, \frac{1}{2}-y, -z\right]$	[5]
6	$\left[\frac{1}{2}-x, y, z+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[11]
12	$\left[\frac{1}{2}-x, -y, z\right]$	[12]
13	$[-x, -y, -z]$	[13]
14	$\left[-x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[14]
15	$\left[x, -y, z+\frac{1}{2}\right]$	[15]
16	$\left[x, y+\frac{1}{2}, -z\right]$	[16]