MSG No. 68.512 $Ccca1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `2221'`

No.	position	mapping
1	$\left[0,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,2,3,4,17,18,19,20]`
2	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[5,6,7,8,21,22,23,24]`
3	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[9,10,11,12,25,26,27,28]`
4	$\left[0,\ \frac{3}{4},\ \frac{3}{4}\right]$	`[13,14,15,16,29,30,31,32]`

Table 2: Wyckoff site: `4b`, site symmetry: `2221'`

No.	position	mapping
1	$\left[0,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[1,2,3,4,17,18,19,20]`
2	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[5,6,7,8,21,22,23,24]`
3	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{3}{4}\right]$	`[9,10,11,12,25,26,27,28]`
4	$\left[0,\ \frac{3}{4},\ \frac{1}{4}\right]$	`[13,14,15,16,29,30,31,32]`

Table 3: Wyckoff site: `8c`, site symmetry: `-11'`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{3}{4},\ 0\right]$	`[1,5,17,21]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[2,6,18,22]`
3	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[3,7,19,23]`
4	$\left[\frac{3}{4},\ \frac{3}{4},\ 0\right]$	`[4,8,20,24]`
5	$\left[\frac{3}{4},\ \frac{1}{4},\ 0\right]$	`[9,13,25,29]`
6	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}\right]$	`[10,14,26,30]`
7	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{2}\right]$	`[11,15,27,31]`
8	$\left[\frac{1}{4},\ \frac{1}{4},\ 0\right]$	`[12,16,28,32]`

Table 4: Wyckoff site: `8d`, site symmetry: `-11'`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,13,17,29]`
2	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[2,14,18,30]`
3	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[3,15,19,31]`
4	$\left[0,\ \frac{1}{2},\ 0\right]$	`[4,16,20,32]`
5	$\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[5,9,21,25]`
6	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[6,10,22,26]`
7	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[7,11,23,27]`
8	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[8,12,24,28]`

Table 5: Wyckoff site: `8e`, site symmetry: `2..1'`

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,2,17,18]`
2	$\left[-x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[3,4,19,20]`
3	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[5,6,21,22]`
4	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[7,8,23,24]`
5	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[9,10,25,26]`
6	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	`[11,12,27,28]`
7	$\left[-x,\ \frac{3}{4},\ \frac{3}{4}\right]$	`[13,14,29,30]`
8	$\left[x,\ \frac{3}{4},\ \frac{3}{4}\right]$	`[15,16,31,32]`

Table 6: Wyckoff site: `8f`, site symmetry: `.2.1'`

No.	position	mapping
1	$\left[0,\ y,\ \frac{1}{4}\right]$	`[1,3,17,19]`
2	$\left[0,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	`[2,4,18,20]`
3	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	`[5,7,21,23]`
4	$\left[\frac{1}{2},\ y,\ \frac{3}{4}\right]$	`[6,8,22,24]`
5	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{4}\right]$	`[9,11,25,27]`
6	$\left[\frac{1}{2},\ -y,\ \frac{1}{4}\right]$	`[10,12,26,28]`
7	$\left[0,\ -y,\ \frac{3}{4}\right]$	`[13,15,29,31]`
8	$\left[0,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	`[14,16,30,32]`

Table 7: Wyckoff site: `8g`, site symmetry: `..21'`

No.	position	mapping
1	$\left[0,\ \frac{1}{4},\ z\right]$	`[1,4,17,20]`
2	$\left[0,\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[2,3,18,19]`
3	$\left[\frac{1}{2},\ \frac{1}{4},\ -z\right]$	`[5,8,21,24]`
4	$\left[\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[6,7,22,23]`
5	$\left[\frac{1}{2},\ \frac{3}{4},\ z\right]$	`[9,12,25,28]`
6	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[10,11,26,27]`
7	$\left[0,\ \frac{3}{4},\ -z\right]$	`[13,16,29,32]`
8	$\left[0,\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[14,15,30,31]`

Table 8: Wyckoff site: `8h`, site symmetry: `..21'`

No.	position	mapping
1	$\left[\frac{1}{4},\ 0,\ z\right]$	`[1,12,17,28]`
2	$\left[\frac{1}{4},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[2,11,18,27]`
3	$\left[\frac{3}{4},\ 0,\ \frac{1}{2}-z\right]$	`[3,10,19,26]`

continued ...

Table 8

No.	position	mapping
4	$\left[\frac{3}{4}, \frac{1}{2}, z\right]$	[4,9,20,25]
5	$\left[\frac{1}{4}, \frac{1}{2}, -z\right]$	[5,16,21,32]
6	$\left[\frac{1}{4}, 0, z+\frac{1}{2}\right]$	[6,15,22,31]
7	$\left[\frac{3}{4}, \frac{1}{2}, z+\frac{1}{2}\right]$	[7,14,23,30]
8	$\left[\frac{3}{4}, 0, -z\right]$	[8,13,24,29]

Table 9: Wyckoff site: 16i, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$\left[x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[2,18]
3	$\left[-x, y, \frac{1}{2}-z\right]$	[3,19]
4	$\left[-x, \frac{1}{2}-y, z\right]$	[4,20]
5	$\left[\frac{1}{2}-x, \frac{1}{2}-y, -z\right]$	[5,21]
6	$\left[\frac{1}{2}-x, y, z+\frac{1}{2}\right]$	[6,22]
7	$\left[x+\frac{1}{2}, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[7,23]
8	$\left[x+\frac{1}{2}, y, -z\right]$	[8,24]
9	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z\right]$	[9,25]
10	$\left[x+\frac{1}{2}, -y, \frac{1}{2}-z\right]$	[10,26]
11	$\left[\frac{1}{2}-x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[11,27]
12	$\left[\frac{1}{2}-x, -y, z\right]$	[12,28]
13	$[-x, -y, -z]$	[13,29]
14	$\left[-x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[14,30]
15	$\left[x, -y, z+\frac{1}{2}\right]$	[15,31]
16	$\left[x, y+\frac{1}{2}, -z\right]$	[16,32]