MSG No. 63.458 $Cmcm1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `2/m..1'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2/m..1'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `m2m1'`

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

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

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `m..1'`

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

Table 7: Wyckoff site: `8g`, site symmetry: `..m1'`

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

Table 8: Wyckoff site: `16h`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$[x, -y, -z]$	[2,18]
3	$\left[-x, y, \frac{1}{2}-z\right]$	[3,19]

continued ...

Table 8

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