MSG No. 74.559 $Imm'a'$ [Type III, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `.2'/m'.`

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `mm'2'`

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

continued ...

Table 5

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

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `.m'.`

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

Table 10: Wyckoff site: `16j`, site symmetry: `1`

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