MSG No. 67.506 $Cmm'a'$ [Type III, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `.2'/m'.`

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

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	`[3,7,9,13]`
4	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	`[4,8,10,14]`

Table 6: Wyckoff site: `4f`, site symmetry: `.2'/m'.`

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

Table 7: Wyckoff site: `4g`, site symmetry: `mm'2'`

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `2..`

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

continued ...

Table 9

No.	position	mapping
4	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[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	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[13,14]`
8	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[15,16]`

Table 10: Wyckoff site: `8j`, site symmetry: `.2'.`

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

Table 11: Wyckoff site: `8k`, site symmetry: `.2'.`

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

Table 12: Wyckoff site: `8l`, site symmetry: `..2'`

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

continued ...

Table 12

No.	position	mapping
7	$\left[\frac{1}{4}, \frac{1}{2}, -z\right]$	`[11,16]`
8	$\left[\frac{1}{4}, \frac{1}{2}, z\right]$	`[12,15]`

Table 13: Wyckoff site: `8m`, site symmetry: `m..`

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

Table 14: Wyckoff site: `8n`, site symmetry: `.m'.`

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

Table 15: Wyckoff site: `16o`, 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	$\left[\frac{1}{2}-x, y, -z\right]$	`[5]`
6	$\left[\frac{1}{2}-x, -y, z\right]$	`[6]`
7	$\left[x+\frac{1}{2}, -y, z\right]$	`[7]`
8	$\left[x+\frac{1}{2}, y, -z\right]$	`[8]`
9	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z\right]$	`[9]`

continued ...

Table 15

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