MSG No. 67.505 $Cm'm'a$ [Type III, orthorhombic]

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

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: `2'2'2`

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	$[0, 0, 0]$	`[1,3,5,7]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[2,4,6,8]`
3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[9,11,13,15]`
4	$\left[0, \frac{1}{2}, 0\right]$	`[10,12,14,16]`

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

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

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

continued ...

Table 9

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

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

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

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

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

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

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

continued ...

Table 12

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

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

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

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

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

Table 15: Wyckoff site: `16o`, site symmetry: `1`

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