MSG No. 67.504 $Cmma'$ [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	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	`[1,6,12,15]`
2	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	`[2,5,11,16]`

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `mm2`

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

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

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

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

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	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[11]
12	$\left[x,\, \frac{1}{2}-y,\, z\right]$	[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	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[15]
16	$\left[x,\, y+\frac{1}{2},\, -z\right]$	[16]