MSG No. 66.496 $Ccc'm'$ [Type III, orthorhombic]

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[3,6,9,16]
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[4,5,10,15]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 12

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

Table 13: Wyckoff site: 16m, site symmetry: 1

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