MSG No. 65.485 $Cm'm'm$ [Type III, orthorhombic]

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

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

Table 2: Wyckoff site: `2b`, site symmetry: `m'm'm`

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

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

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

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

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

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

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

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

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

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

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

Table 8: Wyckoff site: `4h`, site symmetry: `2'm'm`

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

Table 9: Wyckoff site: `4i`, site symmetry: `m'2'm`

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

Table 10: Wyckoff site: `4j`, site symmetry: `m'2'm`

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

Table 11: Wyckoff site: `4k`, site symmetry: `m'm'2`

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

Table 12: Wyckoff site: `4l`, site symmetry: `m'm'2`

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

Table 13: Wyckoff site: `8m`, site symmetry: `..2`

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

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

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

Table 15: Wyckoff site: 8o, site symmetry: .m'.

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

Table 16: Wyckoff site: 8p, site symmetry: ..m

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

Table 17: Wyckoff site: 8q, site symmetry: ..m

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

Table 18: Wyckoff site: 16r, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[-x,\ -y,\ z]$	[2]
3	$[-x,\ -y,\ -z]$	[3]

continued ...

Table 18

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