MSG No. 58.400 P_annm [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `8e`, site symmetry: `..2'`

No.	position	mapping
1	$\left[\frac{3}{4}, 0, z\right]$	`[1,12]`
2	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2} - z\right]$	`[2,11]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: ..2

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

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

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

Table 8: Wyckoff site: 8h, site symmetry: ..m

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

continued ...

Table 8

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

Table 9: Wyckoff site: `16i`, site symmetry: `1`

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