MSG No. 22.45 $F222$ [Type I, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `222`

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

Table 2: Wyckoff site: `4b`, site symmetry: `222`

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

Table 3: Wyckoff site: `4c`, site symmetry: `222`

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

Table 4: Wyckoff site: `4d`, site symmetry: `222`

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

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

No.	position	mapping
1	$[x, 0, 0]$	`[1,2]`
2	$[-x, 0, 0]$	`[3,4]`

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ z\right]$	[1,16]
2	$\left[\frac{1}{4},\ \frac{3}{4},\ -z\right]$	[2,15]
3	$\left[\frac{3}{4},\ \frac{1}{4},\ -z\right]$	[3,14]
4	$\left[\frac{3}{4},\ \frac{3}{4},\ z\right]$	[4,13]
5	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[5,12]

continued ...

Table 8

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

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

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

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

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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

continued ...

Table 11

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