MSG No. 21.44 C_A222 [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

continued ...

Table 8

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

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

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

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

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

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	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[5]
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[6]
7	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[7]
8	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[8]

continued ...

Table 11

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