MSG No. 20.37 C_A222_1 [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `2'22'`

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

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

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

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

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	$\left[-x,\ \frac{1}{4},\ \frac{1}{4}\right]$	[3,12]
4	$\left[-x,\ \frac{3}{4},\ \frac{3}{4}\right]$	[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	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[7,16]
8	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	[8,15]

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

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