MSG No. 20.35 C_c222_1 [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

Table 8: Wyckoff site: 8h, 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	$\left[0,\ y,\ \frac{3}{4}\right]$	[9,11]

continued ...

Table 8

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

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

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

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

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

Table 11: Wyckoff site: 8k, 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	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[3,14]
4	$\left[\frac{3}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[4,13]
5	$\left[\frac{3}{4},\ \frac{3}{4},\ z\right]$	[5,12]
6	$\left[\frac{3}{4},\ \frac{1}{4},\ -z\right]$	[6,11]
7	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[7,10]
8	$\left[\frac{1}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[8,9]

Table 12: Wyckoff site: `16l`, 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]`
9	$\left[x,\, y,\, z+\frac{1}{2}\right]$	`[9]`
10	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	`[10]`
11	$[-x,\, y,\, -z]$	`[11]`
12	$[-x,\, -y,\, z]$	`[12]`
13	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	`[13]`
14	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	`[14]`
15	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	`[15]`
16	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z\right]$	`[16]`