MSG No. 51.300 P_cmma [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `mm2`

No.	position	mapping
1	$\left[\frac{1}{4}, 0, z\right]$	`[1,4,6,7]`
2	$\left[\frac{3}{4}, 0, -z\right]$	`[2,3,5,8]`

continued ...

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry: mm2

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `.m.`

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

Table 10: Wyckoff site: `8j`, site symmetry: `.m.`

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

Table 11: Wyckoff site: `8k`, site symmetry: `m..`

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

Table 12: Wyckoff site: `16l`, site symmetry: `1`

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

continued ...

Table 12

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