MSG No. 49.273 P_ccm [Type IV, orthorhombic]

Table 1: Wyckoff site: `2a`, site symmetry: `m'm'm`

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

Table 2: Wyckoff site: `2b`, site symmetry: `m'm'm`

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

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

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

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

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

Table 5: Wyckoff site: `2e`, site symmetry: `m'm'm`

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

Table 6: Wyckoff site: `2f`, site symmetry: `m'm'm`

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

Table 7: Wyckoff site: 2g, site symmetry: m'm'm'

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: 2'm'm

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

Table 10: Wyckoff site: 4j, site symmetry: 2m'm'

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

Table 11: Wyckoff site: 4k, site symmetry: 2'm'm

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

Table 12: Wyckoff site: 4l, site symmetry: 2m'm'

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

Table 13: Wyckoff site: 4m, site symmetry: m'2'm

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

Table 14: Wyckoff site: 4n, site symmetry: m'2m'

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

Table 15: Wyckoff site: 4o, site symmetry: m'2'm

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

Table 16: Wyckoff site: 4p, site symmetry: m'2m'

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

Table 17: Wyckoff site: `4q`, site symmetry: `m'm'2`

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

Table 18: Wyckoff site: `4r`, site symmetry: `m'm'2`

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

Table 19: Wyckoff site: `4s`, site symmetry: `m'm'2`

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

Table 20: Wyckoff site: `4t`, site symmetry: `m'm'2`

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

Table 21: Wyckoff site: `8u`, site symmetry: `m'..`

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,14]`
2	$\left[0,\ -y,\ \frac{1}{2}-z\right]$	`[2,13]`
3	$\left[0,\ y,\ \frac{1}{2}-z\right]$	`[3,16]`
4	$[0,\ -y,\ z]$	`[4,15]`

continued ...

Table 21

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

Table 22: Wyckoff site: `8v`, site symmetry: `m'..`

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

Table 23: Wyckoff site: `8w`, site symmetry: `.m'.`

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

Table 24: Wyckoff site: `8x`, site symmetry: `.m'.`

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

continued ...

Table 24

No.	position	mapping
8	$\left[x,\ \frac{1}{2},\ -z\right]$	[8,10]

Table 25: Wyckoff site: 8y, site symmetry: ..m

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

Table 26: Wyckoff site: 8z, site symmetry: ..m'

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

Table 27: Wyckoff site: 16A, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	[2]
3	$\left[-x,\ y,\ \frac{1}{2}-z\right]$	[3]
4	$[-x,\ -y,\ z]$	[4]
5	$[-x,\ -y,\ -z]$	[5]
6	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	[6]
7	$\left[x,\ -y,\ z+\frac{1}{2}\right]$	[7]
8	$[x,\ y,\ -z]$	[8]
9	$\left[x,\ y,\ z+\frac{1}{2}\right]$	[9]
10	$[x,\ -y,\ -z]$	[10]

continued ...

Table 27

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