MSG No. 59.415 P_Cmmn [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `..2'/m'`

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

Table 6: Wyckoff site: `4f`, site symmetry: `..2'/m'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `2'mm'`

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

Table 8: Wyckoff site: `4h`, site symmetry: `2'mm'`

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

Table 9: Wyckoff site: `4i`, site symmetry: `m2'm'`

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

Table 10: Wyckoff site: `4j`, site symmetry: `m2'm'`

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

Table 11: Wyckoff site: 4k, site symmetry: mm2

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

Table 12: Wyckoff site: 4l, site symmetry: mm2

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

Table 13: Wyckoff site: 8m, site symmetry: ..2'

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

Table 14: Wyckoff site: 8n, 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	$\left[\frac{3}{4}, y+\frac{1}{2}, -z\right]$	[3,8]
4	$\left[\frac{1}{4}, \frac{1}{2}-y, z\right]$	[4,7]
5	$\left[\frac{3}{4}, y+\frac{1}{2}, z\right]$	[9,14]
6	$\left[\frac{1}{4}, \frac{1}{2}-y, -z\right]$	[10,13]
7	$\left[\frac{1}{4}, y, -z\right]$	[11,16]
8	$\left[\frac{3}{4}, -y, z\right]$	[12,15]

Table 15: Wyckoff site: 8o, site symmetry: .m.

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

Table 16: Wyckoff site: 8p, site symmetry: ..m'

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

Table 17: Wyckoff site: 8q, site symmetry: ..m'

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

Table 18: Wyckoff site: 16r, site symmetry: 1

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

continued ...

Table 18

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