MSG No. 58.401 P_cnnm [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: `8g`, site symmetry: `..m`

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

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

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

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: 1

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