MSG No. 54.348 P_ccca [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 12

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