MSG No. 49.274 P_Bccm [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `222`

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

Table 2: Wyckoff site: `4b`, site symmetry: `222`

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `..2`

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

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: 2..

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

Table 11: Wyckoff site: 8k, site symmetry: 2..

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

Table 12: Wyckoff site: 8l, site symmetry: .2.

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

continued ...

Table 12

No.	position	mapping
7	$\left[\frac{1}{2}, -y, \frac{1}{4}\right]$	[13,15]
8	$\left[\frac{1}{2}, y, \frac{1}{4}\right]$	[14,16]

Table 13: Wyckoff site: 8m, 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	$\left[x+\frac{1}{2}, y, \frac{1}{2}\right]$	[9,16]
6	$\left[x+\frac{1}{2}, -y, 0\right]$	[10,15]
7	$\left[\frac{1}{2}-x, y, 0\right]$	[11,14]
8	$\left[\frac{1}{2}-x, -y, \frac{1}{2}\right]$	[12,13]

Table 14: Wyckoff site: 8n, site symmetry: m'..

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

Table 15: Wyckoff site: 16o, 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	$\left[x+\frac{1}{2}, y, z+\frac{1}{2}\right]$	[9]

continued ...

Table 15

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