MSG No. 53.334 P_Bmna [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff site: `4i`, site symmetry: `mm'2'`

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

Table 10: Wyckoff site: `4j`, site symmetry: `mm'2'`

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

Table 11: Wyckoff site: `4k`, site symmetry: `m2'm'`

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

Table 12: Wyckoff site: `4l`, site symmetry: `m2'm'`

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 18

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