MSG No. 59.414 P_Bmmn [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: `4c`, 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	$\left[\frac{3}{4}, \frac{1}{4}, z+\frac{1}{2}\right]$	`[9,12,14,15]`
4	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}-z\right]$	`[10,11,13,16]`

Table 4: Wyckoff site: `8d`, site symmetry: `-1`

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

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

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

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

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

Table 8: Wyckoff site: `16h`, 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 8

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	$\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[9]
10	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	[10]
11	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[11]
12	$\left[-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[12]
13	$\left[\frac{1}{2}-x,\ -y,\ \frac{1}{2}-z\right]$	[13]
14	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	[14]
15	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[15]
16	$\left[x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[16]