MSG No. 62.454 P_Bnma [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `2'mm'`

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

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

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `..m'`

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

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

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

Table 8: Wyckoff site: `16h`, site symmetry: `1`

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

continued ...

Table 8

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