MSG No. 51.302 P_Bmma [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: mmm'

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

Table 2: Wyckoff site: 2b, site symmetry: mmm'

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

Table 3: Wyckoff site: 2c, site symmetry: mmm'

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

Table 4: Wyckoff site: 2d, site symmetry: mmm'

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

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

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `mm2`

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

Table 8: Wyckoff site: `4h`, site symmetry: `mm2`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 18

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