MSG No. 47.254 P_ammm [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `2e`, site symmetry: `mmm`

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

Table 6: Wyckoff site: `2f`, site symmetry: `m'mm`

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

Table 7: Wyckoff site: 2g, site symmetry: mmm

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

Table 8: Wyckoff site: 2h, site symmetry: m'mm

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

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

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

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

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

Table 11: Wyckoff site: 4k, site symmetry: 2mm

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

Table 12: Wyckoff site: `4l`, site symmetry: `2mm`

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

Table 13: Wyckoff site: `4m`, site symmetry: `m2m`

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

Table 14: Wyckoff site: `4n`, site symmetry: `m2m`

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

Table 15: Wyckoff site: `4o`, site symmetry: `m'2'm`

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

Table 16: Wyckoff site: `4p`, site symmetry: `m'2'm`

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ \frac{1}{2}\right]$	`[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	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}\right]$	`[4,5,10,15]`

Table 17: Wyckoff site: `4q`, site symmetry: `mm2`

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

Table 18: Wyckoff site: `4r`, site symmetry: `mm2`

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

Table 19: Wyckoff site: `4s`, site symmetry: `m'm2'`

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

Table 20: Wyckoff site: `4t`, site symmetry: `m'm2'`

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

Table 21: Wyckoff site: `8u`, site symmetry: `m..`

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,6]`
2	$[0,\ -y,\ -z]$	`[2,5]`
3	$[0,\ y,\ -z]$	`[3,8]`
4	$[0,\ -y,\ z]$	`[4,7]`

continued ...

Table 21

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

Table 22: Wyckoff site: 8v, site symmetry: m'..

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

Table 23: Wyckoff site: 8w, site symmetry: .m.

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

Table 24: Wyckoff site: 8x, site symmetry: .m.

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

continued ...

Table 24

No.	position	mapping
8	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ z\right]$	[12,14]

Table 25: Wyckoff site: 8y, site symmetry: ..m

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

Table 26: Wyckoff site: 8z, site symmetry: ..m

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

Table 27: Wyckoff site: 16A, site symmetry: 1

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

continued ...

Table 27

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