MSG No. 67.510 C_Ammma [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `mmm'`

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	`[1,6,12,15,18,21,27,32]`
2	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	`[2,5,11,16,17,22,28,31]`
3	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	`[3,8,10,13,20,23,25,30]`
4	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	`[4,7,9,14,19,24,26,29]`

Table 2: Wyckoff site: `4b`, site symmetry: `mmm'`

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	`[1,6,12,15,18,21,27,32]`
2	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	`[2,5,11,16,17,22,28,31]`
3	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	`[3,8,10,13,20,23,25,30]`
4	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	`[4,7,9,14,19,24,26,29]`

Table 3: Wyckoff site: `8c`, site symmetry: `.2/m.`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	`[1,3,13,15]`
2	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	`[2,4,14,16]`
3	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	`[5,7,9,11]`
4	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	`[6,8,10,12]`
5	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[17,19,29,31]`
6	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[18,20,30,32]`
7	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[21,23,25,27]`
8	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[22,24,26,28]`

Table 4: Wyckoff site: `8d`, site symmetry: `2/m..`

No.	position	mapping
1	$[0, 0, 0]$	`[1,2,5,6]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[3,4,7,8]`
3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[9,10,13,14]`
4	$\left[0, \frac{1}{2}, 0\right]$	`[11,12,15,16]`
5	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[17,18,21,22]`
6	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[19,20,23,24]`
7	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[25,26,29,30]`
8	$\left[0, 0, \frac{1}{2}\right]$	`[27,28,31,32]`

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

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	`[1,4,29,32]`
2	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	`[2,3,30,31]`
3	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	`[5,8,25,28]`
4	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	`[6,7,26,27]`
5	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	`[9,12,21,24]`
6	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[10,11,22,23]`
7	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[13,16,17,20]`
8	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	`[14,15,18,19]`

Table 6: Wyckoff site: `8f`, site symmetry: `222`

No.	position	mapping
1	$\left[\frac{1}{4}, 0, 0\right]$	`[1,2,3,4]`
2	$\left[\frac{3}{4}, 0, 0\right]$	`[5,6,7,8]`
3	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	`[9,10,11,12]`
4	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	`[13,14,15,16]`
5	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$	`[17,18,19,20]`
6	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$	`[21,22,23,24]`
7	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	`[25,26,27,28]`
8	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[29,30,31,32]`

Table 7: Wyckoff site: `8g`, site symmetry: `m2'm'`

No.	position	mapping
1	$\left[0, y, \frac{3}{4}\right]$	`[1,6,27,32]`
2	$\left[0, -y, \frac{1}{4}\right]$	`[2,5,28,31]`
3	$\left[\frac{1}{2}, y, \frac{1}{4}\right]$	`[3,8,25,30]`
4	$\left[\frac{1}{2}, -y, \frac{3}{4}\right]$	`[4,7,26,29]`
5	$\left[\frac{1}{2}, y+\frac{1}{2}, \frac{3}{4}\right]$	`[9,14,19,24]`
6	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{1}{4}\right]$	`[10,13,20,23]`
7	$\left[0, y+\frac{1}{2}, \frac{1}{4}\right]$	`[11,16,17,22]`
8	$\left[0, \frac{1}{2}-y, \frac{3}{4}\right]$	`[12,15,18,21]`

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

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	`[1,15,18,32]`
2	$\left[x, \frac{3}{4}, \frac{1}{4}\right]$	`[2,16,17,31]`
3	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{1}{4}\right]$	`[3,13,20,30]`

continued ...

Table 8

No.	position	mapping
4	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{3}{4}\right]$	[4,14,19,29]
5	$\left[-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[5,11,22,28]
6	$\left[-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	[6,12,21,27]
7	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{3}{4}\right]$	[7,9,24,26]
8	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{4}\right]$	[8,10,23,25]

Table 9: Wyckoff site: 8i, site symmetry: mm2

No.	position	mapping
1	$\left[0,\ \frac{1}{4},\ z\right]$	[1,6,12,15]
2	$\left[0,\ \frac{3}{4},\ -z\right]$	[2,5,11,16]
3	$\left[\frac{1}{2},\ \frac{1}{4},\ -z\right]$	[3,8,10,13]
4	$\left[\frac{1}{2},\ \frac{3}{4},\ z\right]$	[4,7,9,14]
5	$\left[0,\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[17,22,28,31]
6	$\left[0,\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[18,21,27,32]
7	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[19,24,26,29]
8	$\left[\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[20,23,25,30]

Table 10: Wyckoff site: 16j, site symmetry: ..2

No.	position	mapping
1	$\left[\frac{1}{4},\ 0,\ z\right]$	[1,4]
2	$\left[\frac{1}{4},\ 0,\ -z\right]$	[2,3]
3	$\left[\frac{3}{4},\ 0,\ -z\right]$	[5,8]
4	$\left[\frac{3}{4},\ 0,\ z\right]$	[6,7]
5	$\left[\frac{3}{4},\ \frac{1}{2},\ z\right]$	[9,12]
6	$\left[\frac{3}{4},\ \frac{1}{2},\ -z\right]$	[10,11]
7	$\left[\frac{1}{4},\ \frac{1}{2},\ -z\right]$	[13,16]
8	$\left[\frac{1}{4},\ \frac{1}{2},\ z\right]$	[14,15]
9	$\left[\frac{1}{4},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[17,20]
10	$\left[\frac{1}{4},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[18,19]
11	$\left[\frac{3}{4},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[21,24]
12	$\left[\frac{3}{4},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[22,23]
13	$\left[\frac{3}{4},\ 0,\ z+\frac{1}{2}\right]$	[25,28]
14	$\left[\frac{3}{4},\ 0,\ \frac{1}{2}-z\right]$	[26,27]
15	$\left[\frac{1}{4},\ 0,\ \frac{1}{2}-z\right]$	[29,32]
16	$\left[\frac{1}{4},\ 0,\ z+\frac{1}{2}\right]$	[30,31]

Table 11: Wyckoff site: `16k`, site symmetry: `2..`

No.	position	mapping
1	$[x,\ 0,\ 0]$	`[1,2]`
2	$\left[\frac{1}{2}-x,\ 0,\ 0\right]$	`[3,4]`
3	$[-x,\ 0,\ 0]$	`[5,6]`
4	$\left[x+\frac{1}{2},\ 0,\ 0\right]$	`[7,8]`
5	$\left[x+\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[9,10]`
6	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[11,12]`
7	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ 0\right]$	`[13,14]`
8	$\left[x,\ \frac{1}{2},\ 0\right]$	`[15,16]`
9	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[17,18]`
10	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[19,20]`
11	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[21,22]`
12	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[23,24]`
13	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[25,26]`
14	$\left[-x,\ 0,\ \frac{1}{2}\right]$	`[27,28]`
15	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$	`[29,30]`
16	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[31,32]`

Table 12: Wyckoff site: `16l`, site symmetry: `.2.`

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ 0\right]$	`[1,3]`
2	$\left[\frac{1}{4},\ -y,\ 0\right]$	`[2,4]`
3	$\left[\frac{3}{4},\ -y,\ 0\right]$	`[5,7]`
4	$\left[\frac{3}{4},\ y,\ 0\right]$	`[6,8]`
5	$\left[\frac{3}{4},\ y+\frac{1}{2},\ 0\right]$	`[9,11]`
6	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ 0\right]$	`[10,12]`
7	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ 0\right]$	`[13,15]`
8	$\left[\frac{1}{4},\ y+\frac{1}{2},\ 0\right]$	`[14,16]`
9	$\left[\frac{1}{4},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[17,19]`
10	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[18,20]`
11	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[21,23]`
12	$\left[\frac{3}{4},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[22,24]`
13	$\left[\frac{3}{4},\ y,\ \frac{1}{2}\right]$	`[25,27]`
14	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}\right]$	`[26,28]`
15	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}\right]$	`[29,31]`
16	$\left[\frac{1}{4},\ y,\ \frac{1}{2}\right]$	`[30,32]`

Table 13: Wyckoff site: `16m`, site symmetry: `.m.`

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ z\right]$	`[1,15]`

continued ...

Table 13

No.	position	mapping
2	$\left[x,\ \frac{3}{4},\ -z\right]$	[2,16]
3	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ -z\right]$	[3,13]
4	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ z\right]$	[4,14]
5	$\left[-x,\ \frac{3}{4},\ -z\right]$	[5,11]
6	$\left[-x,\ \frac{1}{4},\ z\right]$	[6,12]
7	$\left[x+\frac{1}{2},\ \frac{3}{4},\ z\right]$	[7,9]
8	$\left[x+\frac{1}{2},\ \frac{1}{4},\ -z\right]$	[8,10]
9	$\left[x,\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[17,31]
10	$\left[x,\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[18,32]
11	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[19,29]
12	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[20,30]
13	$\left[-x,\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[21,27]
14	$\left[-x,\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[22,28]
15	$\left[x+\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[23,25]
16	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[24,26]

Table 14: Wyckoff site: 16n, site symmetry: m..

No.	position	mapping
1	$[0,\ y,\ z]$	[1,6]
2	$[0,\ -y,\ -z]$	[2,5]
3	$\left[\frac{1}{2},\ y,\ -z\right]$	[3,8]
4	$\left[\frac{1}{2},\ -y,\ z\right]$	[4,7]
5	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[9,14]
6	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[10,13]
7	$\left[0,\ y+\frac{1}{2},\ -z\right]$	[11,16]
8	$\left[0,\ \frac{1}{2}-y,\ z\right]$	[12,15]
9	$\left[0,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[17,22]
10	$\left[0,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[18,21]
11	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[19,24]
12	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[20,23]
13	$\left[\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[25,30]
14	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[26,29]
15	$\left[0,\ y,\ \frac{1}{2}-z\right]$	[27,32]
16	$\left[0,\ -y,\ z+\frac{1}{2}\right]$	[28,31]

Table 15: Wyckoff site: 16o, site symmetry: ..m'

No.	position	mapping
1	$\left[x,\ y,\ \frac{3}{4}\right]$	[1,32]
2	$\left[x,\ -y,\ \frac{1}{4}\right]$	[2,31]
3	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{4}\right]$	[3,30]

continued ...

Table 15

No.	position	mapping
4	$\left[\frac{1}{2}-x,\ -y,\ \frac{3}{4}\right]$	[4,29]
5	$\left[-x,\ -y,\ \frac{1}{4}\right]$	[5,28]
6	$\left[-x,\ y,\ \frac{3}{4}\right]$	[6,27]
7	$\left[x+\frac{1}{2},\ -y,\ \frac{3}{4}\right]$	[7,26]
8	$\left[x+\frac{1}{2},\ y,\ \frac{1}{4}\right]$	[8,25]
9	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[9,24]
10	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[10,23]
11	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[11,22]
12	$\left[-x,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[12,21]
13	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[13,20]
14	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[14,19]
15	$\left[x,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[15,18]
16	$\left[x,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[16,17]

Table 16: Wyckoff site: 32p, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[x,\ -y,\ -z]$	[2]
3	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[3]
4	$\left[\frac{1}{2}-x,\ -y,\ z\right]$	[4]
5	$[-x,\ -y,\ -z]$	[5]
6	$[-x,\ y,\ z]$	[6]
7	$\left[x+\frac{1}{2},\ -y,\ z\right]$	[7]
8	$\left[x+\frac{1}{2},\ y,\ -z\right]$	[8]
9	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[9]
10	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[10]
11	$\left[-x,\ y+\frac{1}{2},\ -z\right]$	[11]
12	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	[12]
13	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	[13]
14	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[14]
15	$\left[x,\ \frac{1}{2}-y,\ z\right]$	[15]
16	$\left[x,\ y+\frac{1}{2},\ -z\right]$	[16]
17	$\left[x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[17]
18	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[18]
19	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[19]
20	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[20]
21	$\left[-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[21]
22	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[22]
23	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[23]
24	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[24]
25	$\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[25]
26	$\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[26]
27	$\left[-x,\ y,\ \frac{1}{2}-z\right]$	[27]

continued ...

Table 16

No.	position	mapping
28	$\left[-x,\, -y,\, z+\frac{1}{2}\right]$	[28]
29	$\left[\frac{1}{2}-x,\, -y,\, \frac{1}{2}-z\right]$	[29]
30	$\left[\frac{1}{2}-x,\, y,\, z+\frac{1}{2}\right]$	[30]
31	$\left[x,\, -y,\, z+\frac{1}{2}\right]$	[31]
32	$\left[x,\, y,\, \frac{1}{2}-z\right]$	[32]