MSG No. 65.490 C_Ammm [Type IV, orthorhombic]

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

No.	position	mapping
1	$[0, 0, 0]$	`[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]`
3	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[17,18,19,20,21,22,23,24]`
4	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[25,26,27,28,29,30,31,32]`

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `2'2'2`

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

Table 7: Wyckoff site: `8g`, site symmetry: `2mm`

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

Table 8: Wyckoff site: `8h`, site symmetry: `m2m`

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

continued ...

Table 8

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0, y, z]$	`[1,6]`

continued ...

Table 13

No.	position	mapping
2	$[0,\ -y,\ -z]$	`[2,5]`
3	$[0,\ y,\ -z]$	`[3,8]`
4	$[0,\ -y,\ z]$	`[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	$\left[\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	`[11,16]`
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	`[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	$\left[0,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[19,24]`
12	$\left[0,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[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	$\left[\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	`[27,32]`
16	$\left[\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	`[28,31]`

Table 14: Wyckoff site: `16n`, 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	$\left[x+\frac{1}{2},\ \frac{1}{2},\ z\right]$	`[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]`
8	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ z\right]$	`[12,14]`
9	$\left[x,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[17,23]`
10	$\left[x,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[18,24]`
11	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[19,21]`
12	$\left[-x,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[20,22]`
13	$\left[x+\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[25,31]`
14	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[26,32]`
15	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}-z\right]$	`[27,29]`
16	$\left[\frac{1}{2}-x,\ 0,\ z+\frac{1}{2}\right]$	`[28,30]`

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

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

continued ...

Table 15

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

Table 16: Wyckoff site: 32p, 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	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[9]
10	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[10]
11	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[11]
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[15]
16	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[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	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[19]
20	$\left[-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[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	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[23]
24	$\left[x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[27]

continued ...

Table 16

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