MSG No. 65.488 C_cmmm [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	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[17,18,19,20,21,22,23,24]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[25,26,27,28,29,30,31,32]`

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `mmm'`

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

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

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

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]`

continued ...

Table 5

No.	position	mapping
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	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[17,24,28,29]
6	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[18,23,27,30]
7	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[19,22,26,31]
8	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[20,21,25,32]

Table 6: Wyckoff site: 8f, site symmetry: ..2/m'

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

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	$\left[x, 0, \frac{1}{2}\right]$	[17,18,23,24]
6	$\left[-x, 0, \frac{1}{2}\right]$	[19,20,21,22]
7	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[25,26,31,32]
8	$\left[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}\right]$	[27,28,29,30]

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

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	[1,7,18,24]
2	$\left[x, 0, \frac{3}{4}\right]$	[2,8,17,23]
3	$\left[-x, 0, \frac{3}{4}\right]$	[3,5,20,22]
4	$\left[-x, 0, \frac{1}{4}\right]$	[4,6,19,21]
5	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[9,15,26,32]

continued ...

Table 8

No.	position	mapping
6	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{3}{4}\right]$	`[10,16,25,31]`
7	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[11,13,28,30]`
8	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[12,14,27,29]`

Table 9: Wyckoff site: `8i`, 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]`
4	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	`[10,12,13,15]`
5	$\left[0,\ y,\ \frac{1}{2}\right]$	`[17,19,22,24]`
6	$\left[0,\ -y,\ \frac{1}{2}\right]$	`[18,20,21,23]`
7	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[25,27,30,32]`
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[26,28,29,31]`

Table 10: Wyckoff site: `8j`, site symmetry: `m2'm'`

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

Table 11: Wyckoff site: `8k`, 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	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[17,20,22,23]`
6	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	`[18,19,21,24]`
7	$\left[\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[25,28,30,31]`
8	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[26,27,29,32]`

Table 12: Wyckoff site: `8l`, 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	$\left[\frac{1}{2},\ 0,\ z\right]$	`[9,12,14,15]`
4	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[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 13: Wyckoff site: `16m`, 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	$\left[\frac{1}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[17,28]`
10	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[18,27]`
11	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[19,26]`
12	$\left[\frac{3}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[20,25]`
13	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[21,32]`
14	$\left[\frac{3}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[22,31]`
15	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[23,30]`
16	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[24,29]`

Table 14: Wyckoff site: `16n`, 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]`
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	$\left[0,\ y,\ z+\frac{1}{2}\right]$	`[17,22]`

continued ...

Table 14

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

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

Table 16: Wyckoff site: 16p, 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	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, 0\right]$	[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	$\left[x,\, y,\, \frac{1}{2}\right]$	[17,24]
10	$\left[x,\, -y,\, \frac{1}{2}\right]$	[18,23]
11	$\left[-x,\, y,\, \frac{1}{2}\right]$	[19,22]

continued ...

Table 16

No.	position	mapping
12	$\left[-x,\, -y,\, \frac{1}{2}\right]$	[20,21]
13	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[25,32]
14	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[26,31]
15	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[27,30]
16	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[28,29]

Table 17: Wyckoff site: 16q, site symmetry: ..m'

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

Table 18: Wyckoff site: 32r, 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]

continued ...

Table 18

No.	position	mapping
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	$\left[x,\, y,\, z+\frac{1}{2}\right]$	[17]
18	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	[18]
19	$\left[-x,\, y,\, \frac{1}{2}-z\right]$	[19]
20	$\left[-x,\, -y,\, z+\frac{1}{2}\right]$	[20]
21	$\left[-x,\, -y,\, \frac{1}{2}-z\right]$	[21]
22	$\left[-x,\, y,\, z+\frac{1}{2}\right]$	[22]
23	$\left[x,\, -y,\, z+\frac{1}{2}\right]$	[23]
24	$\left[x,\, y,\, \frac{1}{2}-z\right]$	[24]
25	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[25]
26	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[26]
27	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27]
28	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[28]
29	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[29]
30	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[30]
31	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[31]
32	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[32]