MSG No. 63.466 C_cmcm [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `mm'm'`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `mm'm`

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ 0\right]$	`[1,13,24,28]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ 0\right]$	`[2,14,23,27]`

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: 2m'm'

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

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

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	[1,8,18,23]
2	$\left[x, 0, \frac{3}{4}\right]$	[2,7,17,24]
3	$\left[-x, 0, \frac{1}{4}\right]$	[3,6,20,21]
4	$\left[-x, 0, \frac{3}{4}\right]$	[4,5,19,22]
5	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[9,16,26,31]

continued ...

Table 8

No.	position	mapping
6	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{3}{4}\right]$	`[10,15,25,32]`
7	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[11,14,28,29]`
8	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[12,13,27,30]`

Table 9: Wyckoff site: `8i`, site symmetry: `m2'm'`

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

Table 10: Wyckoff site: `8j`, site symmetry: `m2m`

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

Table 11: Wyckoff site: `8k`, site symmetry: `mm'2'`

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

Table 12: Wyckoff site: `8l`, site symmetry: `mm'2'`

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

Table 13: Wyckoff site: `16m`, site symmetry: `..2'`

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,6]`
2	$[0,\ -y,\ -z]$	`[2,5]`
3	$\left[0,\ y,\ \frac{1}{2}-z\right]$	`[3,8]`
4	$\left[0,\ -y,\ z+\frac{1}{2}\right]$	`[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	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[11,16]`
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[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	$[0,\, y,\, -z]$	[19,24]
12	$[0,\, -y,\, z]$	[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	$\left[\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[27,32]
16	$\left[\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[28,31]

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

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

Table 16: Wyckoff site: 16p, site symmetry: ..m'

No.	position	mapping
1	$[x,\, y,\, 0]$	[1,24]
2	$[x,\, -y,\, 0]$	[2,23]
3	$\left[-x,\, y,\, \frac{1}{2}\right]$	[3,22]
4	$\left[-x,\, -y,\, \frac{1}{2}\right]$	[4,21]
5	$[-x,\, -y,\, 0]$	[5,20]
6	$[-x,\, y,\, 0]$	[6,19]
7	$\left[x,\, -y,\, \frac{1}{2}\right]$	[7,18]
8	$\left[x,\, y,\, \frac{1}{2}\right]$	[8,17]
9	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, 0\right]$	[9,32]
10	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, 0\right]$	[10,31]
11	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[11,30]

continued ...

Table 16

No.	position	mapping
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[12,29]
13	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ 0\right]$	[13,28]
14	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	[14,27]
15	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[15,26]
16	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[16,25]

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

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

Table 18: Wyckoff site: 32r, site symmetry: 1

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