MSG No. 67.508 C_cmma [Type IV, orthorhombic]

Table 1: Wyckoff site: `8a`, 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	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[17,18,19,20]`
6	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	`[21,22,23,24]`
7	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$	`[25,26,27,28]`
8	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$	`[29,30,31,32]`

Table 2: Wyckoff site: `8b`, site symmetry: `2'2'2`

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

Table 3: Wyckoff site: `8c`, 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	$\left[0, 0, \frac{1}{2}\right]$	`[17,18,21,22]`
6	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[19,20,23,24]`
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[25,26,29,30]`
8	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[27,28,31,32]`

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

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

Table 5: Wyckoff site: `8e`, 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	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{2}\right]$	`[17,19,29,31]`
6	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[18,20,30,32]`
7	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[21,23,25,27]`
8	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}\right]$	`[22,24,26,28]`

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

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

Table 7: Wyckoff site: `8g`, 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]`

continued ...

Table 7

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

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

Table 9: Wyckoff site: 16i, site symmetry: 2'..

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

continued ...

Table 9

No.	position	mapping
14	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{4}\right]$	[14,29]
15	$\left[x,\ \frac{1}{2},\ \frac{1}{4}\right]$	[15,32]
16	$\left[x,\ \frac{1}{2},\ \frac{3}{4}\right]$	[16,31]

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

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

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

continued ...

Table 11

No.	position	mapping
16	$\left[\frac{1}{4},\, y+\frac{1}{2},\, \frac{3}{4}\right]$	[16,30]

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

Table 13: Wyckoff site: 16m, 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	$\left[0,\, y,\, z+\frac{1}{2}\right]$	[17,22]
10	$\left[0,\, -y,\, \frac{1}{2}-z\right]$	[18,21]
11	$\left[\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[19,24]
12	$\left[\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[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	$\left[0,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27,32]
16	$\left[0,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[28,31]

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

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

Table 15: Wyckoff site: `32o`, 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	$\left[x,\ y,\ z+\frac{1}{2}\right]$	`[17]`
18	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	`[18]`
19	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	`[19]`
20	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	`[20]`
21	$\left[-x,\ -y,\ \frac{1}{2}-z\right]$	`[21]`
22	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	`[22]`
23	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	`[23]`

continued ...

Table 15

No.	position	mapping
24	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[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	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27]
28	$\left[-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[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	$\left[x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[31]
32	$\left[x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[32]