MSG No. 42.223 F_Smm2 [Type IV, orthorhombic]

Table 1: Wyckoff site: 8a, site symmetry: mm2

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: m'm2'

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

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

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

Table 5: Wyckoff site: `16e`, site symmetry: `.m.`

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

Table 6: Wyckoff site: `16f`, site symmetry: `.m'.`

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

continued …

Table 6

No.	position	mapping
10	$\left[\frac{1}{2}-x, \frac{3}{4}, z+\frac{1}{2}\right]$	[10,31]
11	$\left[\frac{1}{2}-x, \frac{1}{4}, z+\frac{1}{2}\right]$	[11,30]
12	$\left[x+\frac{1}{2}, \frac{3}{4}, z+\frac{1}{2}\right]$	[12,29]
13	$\left[x+\frac{1}{2}, \frac{3}{4}, z\right]$	[13,28]
14	$\left[\frac{1}{2}-x, \frac{1}{4}, z\right]$	[14,27]
15	$\left[\frac{1}{2}-x, \frac{3}{4}, z\right]$	[15,26]
16	$\left[x+\frac{1}{2}, \frac{1}{4}, z\right]$	[16,25]

Table 7: Wyckoff site: `16g`, site symmetry: `m..`

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

Table 8: Wyckoff site: `16h`, site symmetry: `m'..`

No.	position	mapping
1	$\left[\frac{1}{4}, y, z\right]$	[1,27]
2	$\left[\frac{3}{4}, -y, z\right]$	[2,28]
3	$\left[\frac{3}{4}, y, z\right]$	[3,25]
4	$\left[\frac{1}{4}, -y, z\right]$	[4,26]
5	$\left[\frac{1}{4}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[5,31]
6	$\left[\frac{3}{4}, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[6,32]
7	$\left[\frac{3}{4}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[7,29]
8	$\left[\frac{1}{4}, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[8,30]
9	$\left[\frac{3}{4}, y, z+\frac{1}{2}\right]$	[9,19]
10	$\left[\frac{1}{4}, -y, z+\frac{1}{2}\right]$	[10,20]
11	$\left[\frac{1}{4}, y, z+\frac{1}{2}\right]$	[11,17]

Table 8

No.	position	mapping
12	$\left[\frac{3}{4},\, -y,\, z+\frac{1}{2}\right]$	[12,18]
13	$\left[\frac{3}{4},\, y+\frac{1}{2},\, z\right]$	[13,23]
14	$\left[\frac{1}{4},\, \frac{1}{2}-y,\, z\right]$	[14,24]
15	$\left[\frac{1}{4},\, y+\frac{1}{2},\, z\right]$	[15,21]
16	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, z\right]$	[16,22]

Table 9: Wyckoff site: 32i, 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	$\left[x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[5]
6	$\left[-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[6]
7	$\left[-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[7]
8	$\left[x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[8]
9	$\left[x+\frac{1}{2},\, y,\, z+\frac{1}{2}\right]$	[9]
10	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[10]
11	$\left[\frac{1}{2}-x,\, y,\, z+\frac{1}{2}\right]$	[11]
12	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[12]
13	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z\right]$	[13]
14	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z\right]$	[14]
15	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[15]
16	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[16]
17	$\left[x,\, y,\, z+\frac{1}{2}\right]$	[17]
18	$\left[-x,\, -y,\, z+\frac{1}{2}\right]$	[18]
19	$\left[-x,\, y,\, z+\frac{1}{2}\right]$	[19]
20	$\left[x,\, -y,\, z+\frac{1}{2}\right]$	[20]
21	$\left[x,\, y+\frac{1}{2},\, z\right]$	[21]
22	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	[22]
23	$\left[-x,\, y+\frac{1}{2},\, z\right]$	[23]
24	$\left[x,\, \frac{1}{2}-y,\, z\right]$	[24]
25	$\left[x+\frac{1}{2},\, y,\, z\right]$	[25]
26	$\left[\frac{1}{2}-x,\, -y,\, z\right]$	[26]
27	$\left[\frac{1}{2}-x,\, y,\, z\right]$	[27]
28	$\left[x+\frac{1}{2},\, -y,\, z\right]$	[28]
29	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[29]
30	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[30]
31	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[31]
32	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[32]