MSG No. 69.523 $Fm'mm$ [Type III, orthorhombic]

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

No.	position	mapping
1	$[0, 0, 0]$	`[1,2,3,4,5,6,7,8]`
2	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[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	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[25,26,27,28,29,30,31,32]`

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

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	`[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	$\left[\frac{1}{2}, 0, 0\right]$	`[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 3: Wyckoff site: `8c`, site symmetry: `2/m'..`

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

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

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `22'2'`

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

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

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

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

No.	position	mapping
1	$[0, y, 0]$	`[1,4,5,8]`
2	$[0, -y, 0]$	`[2,3,6,7]`
3	$\left[0, y+\frac{1}{2}, \frac{1}{2}\right]$	`[9,12,13,16]`

continued ...

Table 8

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0, y, z]$	`[1,8]`

continued ...

Table 13

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

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

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

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

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,4]`
2	$[x,\ -y,\ 0]$	`[2,3]`
3	$[-x,\ y,\ 0]$	`[5,8]`

continued ...

Table 15

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

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	$\left[x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[9]
10	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[10]
11	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[11]
12	$\left[x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[12]
13	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[13]
14	$\left[-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[14]
15	$\left[-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[15]
16	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[16]
17	$\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[17]
18	$\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[18]
19	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[19]
20	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[20]
21	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	[22]
23	$\left[\frac{1}{2}-x,\ -y,\ \frac{1}{2}-z\right]$	[23]
24	$\left[\frac{1}{2}-x,\ y,\ z+\frac{1}{2}\right]$	[24]
25	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[25]
26	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[26]
27	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[27]

continued ...

Table 16

No.	position	mapping
28	$\left[x+\frac{1}{2}, y+\frac{1}{2}, -z\right]$	[28]
29	$\left[\frac{1}{2}-x, y+\frac{1}{2}, -z\right]$	[29]
30	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z\right]$	[30]
31	$\left[\frac{1}{2}-x, \frac{1}{2}-y, -z\right]$	[31]
32	$\left[\frac{1}{2}-x, y+\frac{1}{2}, z\right]$	[32]