MSG No. 69.522 $Fmmm1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `mmm1'`

No.	position	mapping
1	$[0, 0, 0]$	`[1,2,3,4,5,6,7,8,33,34,35,36,37,38,39,40]`
2	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[9,10,11,12,13,14,15,16,41,42,43,44,45,46,47,48]`
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[17,18,19,20,21,22,23,24,49,50,51,52,53,54,55,56]`
4	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[25,26,27,28,29,30,31,32,57,58,59,60,61,62,63,64]`

Table 2: Wyckoff site: `4b`, site symmetry: `mmm1'`

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	`[1,2,3,4,5,6,7,8,33,34,35,36,37,38,39,40]`
2	$\left[0, \frac{1}{2}, 0\right]$	`[9,10,11,12,13,14,15,16,41,42,43,44,45,46,47,48]`
3	$\left[\frac{1}{2}, 0, 0\right]$	`[17,18,19,20,21,22,23,24,49,50,51,52,53,54,55,56]`
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[25,26,27,28,29,30,31,32,57,58,59,60,61,62,63,64]`

Table 3: Wyckoff site: `8c`, site symmetry: `2/m..1'`

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	`[1,6,10,13,33,38,42,45]`
2	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	`[2,5,9,14,34,37,41,46]`
3	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	`[3,8,12,15,35,40,44,47]`
4	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	`[4,7,11,16,36,39,43,48]`
5	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	`[17,22,26,29,49,54,58,61]`
6	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	`[18,21,25,30,50,53,57,62]`
7	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	`[19,24,28,31,51,56,60,63]`
8	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	`[20,23,27,32,52,55,59,64]`

Table 4: Wyckoff site: `8d`, site symmetry: `.2/m.1'`

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	`[1,7,19,21,33,39,51,53]`
2	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	`[2,8,20,22,34,40,52,54]`
3	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	`[3,5,17,23,35,37,49,55]`
4	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	`[4,6,18,24,36,38,50,56]`
5	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	`[9,15,27,29,41,47,59,61]`
6	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[10,16,28,30,42,48,60,62]`
7	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[11,13,25,31,43,45,57,63]`
8	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	`[12,14,26,32,44,46,58,64]`

Table 5: Wyckoff site: `8e`, site symmetry: `..2/m1'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	`[1,8,28,29,33,40,60,61]`
2	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	`[2,7,27,30,34,39,59,62]`
3	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	`[3,6,26,31,35,38,58,63]`
4	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	`[4,5,25,32,36,37,57,64]`
5	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[9,16,20,21,41,48,52,53]`
6	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[10,15,19,22,42,47,51,54]`
7	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[11,14,18,23,43,46,50,55]`
8	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[12,13,17,24,44,45,49,56]`

Table 6: Wyckoff site: `8f`, site symmetry: `2221'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,10,19,28,33,42,51,60]`
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[2,9,20,27,34,41,52,59]`
3	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[3,12,17,26,35,44,49,58]`
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[4,11,18,25,36,43,50,57]`
5	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[5,14,23,32,37,46,55,64]`
6	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[6,13,24,31,38,45,56,63]`
7	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[7,16,21,30,39,48,53,62]`
8	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[8,15,22,29,40,47,54,61]`

Table 7: Wyckoff site: `8g`, site symmetry: `2mm1'`

No.	position	mapping
1	$[x, 0, 0]$	`[1,2,7,8,33,34,39,40]`
2	$[-x, 0, 0]$	`[3,4,5,6,35,36,37,38]`
3	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	`[9,10,15,16,41,42,47,48]`
4	$\left[-x, \frac{1}{2}, \frac{1}{2}\right]$	`[11,12,13,14,43,44,45,46]`
5	$\left[x+\frac{1}{2}, 0, \frac{1}{2}\right]$	`[17,18,23,24,49,50,55,56]`
6	$\left[\frac{1}{2}-x, 0, \frac{1}{2}\right]$	`[19,20,21,22,51,52,53,54]`
7	$\left[x+\frac{1}{2}, \frac{1}{2}, 0\right]$	`[25,26,31,32,57,58,63,64]`
8	$\left[\frac{1}{2}-x, \frac{1}{2}, 0\right]$	`[27,28,29,30,59,60,61,62]`

Table 8: Wyckoff site: `8h`, site symmetry: `m2m1'`

No.	position	mapping
1	$[0, y, 0]$	`[1,3,6,8,33,35,38,40]`
2	$[0, -y, 0]$	`[2,4,5,7,34,36,37,39]`
3	$\left[0, y+\frac{1}{2}, \frac{1}{2}\right]$	`[9,11,14,16,41,43,46,48]`

continued ...

Table 8

No.	position	mapping
4	$\left[0,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[10,12,13,15,42,44,45,47]`
5	$\left[\frac{1}{2},\ y,\ \frac{1}{2}\right]$	`[17,19,22,24,49,51,54,56]`
6	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}\right]$	`[18,20,21,23,50,52,53,55]`
7	$\left[\frac{1}{2},\ y+\frac{1}{2},\ 0\right]$	`[25,27,30,32,57,59,62,64]`
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	`[26,28,29,31,58,60,61,63]`

Table 9: Wyckoff site: `8i`, site symmetry: `mm21'`

No.	position	mapping
1	$[0,\ 0,\ z]$	`[1,4,6,7,33,36,38,39]`
2	$[0,\ 0,\ -z]$	`[2,3,5,8,34,35,37,40]`
3	$\left[0,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[9,12,14,15,41,44,46,47]`
4	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[10,11,13,16,42,43,45,48]`
5	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[17,20,22,23,49,52,54,55]`
6	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[18,19,21,24,50,51,53,56]`
7	$\left[\frac{1}{2},\ \frac{1}{2},\ z\right]$	`[25,28,30,31,57,60,62,63]`
8	$\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$	`[26,27,29,32,58,59,61,64]`

Table 10: Wyckoff site: `16j`, site symmetry: `..21'`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ z\right]$	`[1,28,33,60]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ -z\right]$	`[2,27,34,59]`
3	$\left[\frac{3}{4},\ \frac{1}{4},\ -z\right]$	`[3,26,35,58]`
4	$\left[\frac{3}{4},\ \frac{3}{4},\ z\right]$	`[4,25,36,57]`
5	$\left[\frac{3}{4},\ \frac{3}{4},\ -z\right]$	`[5,32,37,64]`
6	$\left[\frac{3}{4},\ \frac{1}{4},\ z\right]$	`[6,31,38,63]`
7	$\left[\frac{1}{4},\ \frac{3}{4},\ z\right]$	`[7,30,39,62]`
8	$\left[\frac{1}{4},\ \frac{1}{4},\ -z\right]$	`[8,29,40,61]`
9	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[9,20,41,52]`
10	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[10,19,42,51]`
11	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[11,18,43,50]`
12	$\left[\frac{3}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[12,17,44,49]`
13	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[13,24,45,56]`
14	$\left[\frac{3}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[14,23,46,55]`
15	$\left[\frac{1}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[15,22,47,54]`
16	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[16,21,48,53]`

Table 11: Wyckoff site: `16k`, site symmetry: `.2.1'`

No.	position	mapping
1	$\left[\frac{1}{4}, y, \frac{1}{4}\right]$	`[1,19,33,51]`
2	$\left[\frac{1}{4}, -y, \frac{3}{4}\right]$	`[2,20,34,52]`
3	$\left[\frac{3}{4}, y, \frac{3}{4}\right]$	`[3,17,35,49]`
4	$\left[\frac{3}{4}, -y, \frac{1}{4}\right]$	`[4,18,36,50]`
5	$\left[\frac{3}{4}, -y, \frac{3}{4}\right]$	`[5,23,37,55]`
6	$\left[\frac{3}{4}, y, \frac{1}{4}\right]$	`[6,24,38,56]`
7	$\left[\frac{1}{4}, -y, \frac{1}{4}\right]$	`[7,21,39,53]`
8	$\left[\frac{1}{4}, y, \frac{3}{4}\right]$	`[8,22,40,54]`
9	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{3}{4}\right]$	`[9,27,41,59]`
10	$\left[\frac{1}{4}, \frac{1}{2}-y, \frac{1}{4}\right]$	`[10,28,42,60]`
11	$\left[\frac{3}{4}, y+\frac{1}{2}, \frac{1}{4}\right]$	`[11,25,43,57]`
12	$\left[\frac{3}{4}, \frac{1}{2}-y, \frac{3}{4}\right]$	`[12,26,44,58]`
13	$\left[\frac{3}{4}, \frac{1}{2}-y, \frac{1}{4}\right]$	`[13,31,45,63]`
14	$\left[\frac{3}{4}, y+\frac{1}{2}, \frac{3}{4}\right]$	`[14,32,46,64]`
15	$\left[\frac{1}{4}, \frac{1}{2}-y, \frac{3}{4}\right]$	`[15,29,47,61]`
16	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{1}{4}\right]$	`[16,30,48,62]`

Table 12: Wyckoff site: `16l`, site symmetry: `2..1'`

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	`[1,10,33,42]`
2	$\left[x, \frac{3}{4}, \frac{3}{4}\right]$	`[2,9,34,41]`
3	$\left[-x, \frac{1}{4}, \frac{3}{4}\right]$	`[3,12,35,44]`
4	$\left[-x, \frac{3}{4}, \frac{1}{4}\right]$	`[4,11,36,43]`
5	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	`[5,14,37,46]`
6	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	`[6,13,38,45]`
7	$\left[x, \frac{3}{4}, \frac{1}{4}\right]$	`[7,16,39,48]`
8	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	`[8,15,40,47]`
9	$\left[x+\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	`[17,26,49,58]`
10	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	`[18,25,50,57]`
11	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{1}{4}\right]$	`[19,28,51,60]`
12	$\left[\frac{1}{2}-x, \frac{3}{4}, \frac{3}{4}\right]$	`[20,27,52,59]`
13	$\left[\frac{1}{2}-x, \frac{3}{4}, \frac{1}{4}\right]$	`[21,30,53,62]`
14	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{3}{4}\right]$	`[22,29,54,61]`
15	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	`[23,32,55,64]`
16	$\left[x+\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	`[24,31,56,63]`

Table 13: Wyckoff site: `16m`, site symmetry: `m..1'`

No.	position	mapping
1	$[0, y, z]$	`[1,6,33,38]`

continued ...

Table 13

No.	position	mapping
2	$[0,\ -y,\ -z]$	`[2,5,34,37]`
3	$[0,\ y,\ -z]$	`[3,8,35,40]`
4	$[0,\ -y,\ z]$	`[4,7,36,39]`
5	$\left[0,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[9,14,41,46]`
6	$\left[0,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	`[10,13,42,45]`
7	$\left[0,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[11,16,43,48]`
8	$\left[0,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[12,15,44,47]`
9	$\left[\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	`[17,22,49,54]`
10	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	`[18,21,50,53]`
11	$\left[\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	`[19,24,51,56]`
12	$\left[\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	`[20,23,52,55]`
13	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	`[25,30,57,62]`
14	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	`[26,29,58,61]`
15	$\left[\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	`[27,32,59,64]`
16	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	`[28,31,60,63]`

Table 14: Wyckoff site: `16n`, site symmetry: `.m.1'`

No.	position	mapping
1	$[x,\ 0,\ z]$	`[1,7,33,39]`
2	$[x,\ 0,\ -z]$	`[2,8,34,40]`
3	$[-x,\ 0,\ -z]$	`[3,5,35,37]`
4	$[-x,\ 0,\ z]$	`[4,6,36,38]`
5	$\left[x,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[9,15,41,47]`
6	$\left[x,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[10,16,42,48]`
7	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[11,13,43,45]`
8	$\left[-x,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[12,14,44,46]`
9	$\left[x+\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[17,23,49,55]`
10	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[18,24,50,56]`
11	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}-z\right]$	`[19,21,51,53]`
12	$\left[\frac{1}{2}-x,\ 0,\ z+\frac{1}{2}\right]$	`[20,22,52,54]`
13	$\left[x+\frac{1}{2},\ \frac{1}{2},\ z\right]$	`[25,31,57,63]`
14	$\left[x+\frac{1}{2},\ \frac{1}{2},\ -z\right]$	`[26,32,58,64]`
15	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ -z\right]$	`[27,29,59,61]`
16	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ z\right]$	`[28,30,60,62]`

Table 15: Wyckoff site: `16o`, site symmetry: `..m1'`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,8,33,40]`
2	$[x,\ -y,\ 0]$	`[2,7,34,39]`
3	$[-x,\ y,\ 0]$	`[3,6,35,38]`

continued ...

Table 15

No.	position	mapping
4	$[-x,\, -y,\, 0]$	[4,5,36,37]
5	$\left[x,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[9,16,41,48]
6	$\left[x,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[10,15,42,47]
7	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[11,14,43,46]
8	$\left[-x,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[12,13,44,45]
9	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}\right]$	[17,24,49,56]
10	$\left[x+\frac{1}{2},\, -y,\, \frac{1}{2}\right]$	[18,23,50,55]
11	$\left[\frac{1}{2}-x,\, y,\, \frac{1}{2}\right]$	[19,22,51,54]
12	$\left[\frac{1}{2}-x,\, -y,\, \frac{1}{2}\right]$	[20,21,52,53]
13	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, 0\right]$	[25,32,57,64]
14	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, 0\right]$	[26,31,58,63]
15	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, 0\right]$	[27,30,59,62]
16	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, 0\right]$	[28,29,60,61]

Table 16: Wyckoff site: 32p, site symmetry: 11'

No.	position	mapping
1	$[x,\, y,\, z]$	[1,33]
2	$[x,\, -y,\, -z]$	[2,34]
3	$[-x,\, y,\, -z]$	[3,35]
4	$[-x,\, -y,\, z]$	[4,36]
5	$[-x,\, -y,\, -z]$	[5,37]
6	$[-x,\, y,\, z]$	[6,38]
7	$[x,\, -y,\, z]$	[7,39]
8	$[x,\, y,\, -z]$	[8,40]
9	$\left[x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[9,41]
10	$\left[x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[10,42]
11	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[11,43]
12	$\left[-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[12,44]
13	$\left[-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[13,45]
14	$\left[-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[14,46]
15	$\left[x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[15,47]
16	$\left[x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[16,48]
17	$\left[x+\frac{1}{2},\, y,\, z+\frac{1}{2}\right]$	[17,49]
18	$\left[x+\frac{1}{2},\, -y,\, \frac{1}{2}-z\right]$	[18,50]
19	$\left[\frac{1}{2}-x,\, y,\, \frac{1}{2}-z\right]$	[19,51]
20	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[20,52]
21	$\left[\frac{1}{2}-x,\, -y,\, \frac{1}{2}-z\right]$	[21,53]
22	$\left[\frac{1}{2}-x,\, y,\, z+\frac{1}{2}\right]$	[22,54]
23	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[23,55]
24	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[24,56]
25	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z\right]$	[25,57]
26	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[26,58]
27	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[27,59]

continued ...

Table 16

No.	position	mapping
28	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[28,60]
29	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	[29,61]
30	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[30,62]
31	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[31,63]
32	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[32,64]