MSG No. 69.521 $Fmmm$ [Type I, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: mmm

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: mmm

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	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[1,6,10,13]
2	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[2,5,9,14]
3	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[3,8,12,15]
4	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[4,7,11,16]
5	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[17,22,26,29]
6	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[18,21,25,30]
7	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[19,24,28,31]
8	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[20,23,27,32]

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

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `222`

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

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

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

Table 8: Wyckoff site: `8h`, site symmetry: `m2m`

No.	position	mapping
1	$[0, y, 0]$	`[1,3,6,8]`
2	$[0, -y, 0]$	`[2,4,5,7]`
3	$\left[0, y + \frac{1}{2}, \frac{1}{2}\right]$	`[9,11,14,16]`

continued ...

Table 8

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

Table 9: Wyckoff site: 8i, site symmetry: mm2

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

Table 10: Wyckoff site: 16j, 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	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[3,26]
4	$\left[\frac{3}{4}, \frac{3}{4}, z\right]$	[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	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[7,30]
8	$\left[\frac{1}{4}, \frac{1}{4}, -z\right]$	[8,29]
9	$\left[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}\right]$	[9,20]
10	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z\right]$	[10,19]
11	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	[11,18]
12	$\left[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}\right]$	[12,17]
13	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z\right]$	[13,24]
14	$\left[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}\right]$	[14,23]
15	$\left[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}\right]$	[15,22]
16	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	[16,21]

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	$\left[\frac{3}{4}, y, \frac{3}{4}\right]$	[3,17]
4	$\left[\frac{3}{4}, -y, \frac{1}{4}\right]$	[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	$\left[\frac{1}{4}, -y, \frac{1}{4}\right]$	[7,21]
8	$\left[\frac{1}{4}, y, \frac{3}{4}\right]$	[8,22]
9	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{3}{4}\right]$	[9,27]
10	$\left[\frac{1}{4}, \frac{1}{2}-y, \frac{1}{4}\right]$	[10,28]
11	$\left[\frac{3}{4}, y+\frac{1}{2}, \frac{1}{4}\right]$	[11,25]
12	$\left[\frac{3}{4}, \frac{1}{2}-y, \frac{3}{4}\right]$	[12,26]
13	$\left[\frac{3}{4}, \frac{1}{2}-y, \frac{1}{4}\right]$	[13,31]
14	$\left[\frac{3}{4}, y+\frac{1}{2}, \frac{3}{4}\right]$	[14,32]
15	$\left[\frac{1}{4}, \frac{1}{2}-y, \frac{3}{4}\right]$	[15,29]
16	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{1}{4}\right]$	[16,30]

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	$\left[-x, \frac{1}{4}, \frac{3}{4}\right]$	[3,12]
4	$\left[-x, \frac{3}{4}, \frac{1}{4}\right]$	[4,11]
5	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	[5,14]
6	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	[6,13]
7	$\left[x, \frac{3}{4}, \frac{1}{4}\right]$	[7,16]
8	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	[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	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{1}{4}\right]$	[19,28]
12	$\left[\frac{1}{2}-x, \frac{3}{4}, \frac{3}{4}\right]$	[20,27]
13	$\left[\frac{1}{2}-x, \frac{3}{4}, \frac{1}{4}\right]$	[21,30]
14	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{3}{4}\right]$	[22,29]
15	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[23,32]
16	$\left[x+\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[24,31]

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

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

continued ...

4

Table 13

No.	position	mapping
2	$[0, -y, -z]$	[2,5]
3	$[0, y, -z]$	[3,8]
4	$[0, -y, z]$	[4,7]
5	$\left[0, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[9,14]
6	$\left[0, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[10,13]
7	$\left[0, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[11,16]
8	$\left[0, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[12,15]
9	$\left[\frac{1}{2}, y, z + \frac{1}{2}\right]$	[17,22]
10	$\left[\frac{1}{2}, -y, \frac{1}{2} - z\right]$	[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	$\left[\frac{1}{2}, y + \frac{1}{2}, z\right]$	[25,30]
14	$\left[\frac{1}{2}, \frac{1}{2} - y, -z\right]$	[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 14: Wyckoff site: `16n`, site symmetry: `.m.`

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

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

No.	position	mapping
1	$[x, y, 0]$	[1,8]
2	$[x, -y, 0]$	[2,7]
3	$[-x, y, 0]$	[3,6]

Table 15

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

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	$\left[-x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[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	$\left[-x, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[14]
15	$\left[x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[15]
16	$\left[x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[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	$\left[\frac{1}{2} - x, y, \frac{1}{2} - z\right]$	[19]
20	$\left[\frac{1}{2} - x, -y, z + \frac{1}{2}\right]$	[20]
21	$\left[\frac{1}{2} - x, -y, \frac{1}{2} - z\right]$	[21]
22	$\left[\frac{1}{2} - x, y, z + \frac{1}{2}\right]$	[22]
23	$\left[x + \frac{1}{2}, -y, z + \frac{1}{2}\right]$	[23]
24	$\left[x + \frac{1}{2}, y, \frac{1}{2} - z\right]$	[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	$\left[\frac{1}{2} - x, y + \frac{1}{2}, -z\right]$	[27]

continued ...

Table 16

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