MSG No. 139.533 $I4/m'mm$ [Type III, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `4/m'mm`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `m'mm.`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4'm2'`

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

Table 5: Wyckoff site: `4e`, site symmetry: `4mm`

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

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m'2'm.`

No.	position	mapping
1	$[x, 0, 0]$	`[1,6,9,16]`
2	$[0, x, 0]$	`[2,8,11,15]`
3	$[0, -x, 0]$	`[3,7,12,14]`

continued ...

Table 9

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

Table 10: Wyckoff site: `8j`, site symmetry: `m'2'm`.

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,5]`

continued ...

Table 14

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

Table 15: Wyckoff site: 32o, site symmetry: 1

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

continued ...

Table 15

No.	position	mapping
26	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[26]
27	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27]
28	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[28]
29	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[29]
30	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[31]
32	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[32]