MSG No. 139.535 $I4'/mmm'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4'/mmm'

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'/mmm'

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: mmm.

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

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

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m2m.`

No.	position	mapping
1	$[x, 0, 0]$	`[1,2,7,8]`
2	$[-x, 0, 0]$	`[3,4,5,6]`
3	$[0, x, 0]$	`[9,11,14,16]`

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: m2m.

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

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	$\left[x, \frac{1}{2}-x, \frac{3}{4}\right]$	[2,26]
3	$\left[-x, x+\frac{1}{2}, \frac{3}{4}\right]$	[3,25]
4	$\left[-x, \frac{1}{2}-x, \frac{1}{4}\right]$	[4,28]
5	$\left[-x, \frac{1}{2}-x, \frac{3}{4}\right]$	[5,31]
6	$\left[-x, x+\frac{1}{2}, \frac{1}{4}\right]$	[6,30]
7	$\left[x, \frac{1}{2}-x, \frac{1}{4}\right]$	[7,29]
8	$\left[x, x+\frac{1}{2}, \frac{3}{4}\right]$	[8,32]
9	$\left[\frac{1}{2}-x, x, \frac{1}{4}\right]$	[9,19]
10	$\left[x+\frac{1}{2}, -x, \frac{1}{4}\right]$	[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	$\left[\frac{1}{2}-x, x, \frac{3}{4}\right]$	[14,22]
15	$\left[\frac{1}{2}-x, -x, \frac{1}{4}\right]$	[15,21]
16	$\left[x+\frac{1}{2}, x, \frac{1}{4}\right]$	[16,24]

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

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

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

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

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

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

continued ...

Table 14

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

Table 15: Wyckoff site: 32o, 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	$[-y, x, z]$	[9]
10	$[y, -x, z]$	[10]
11	$[y, x, -z]$	[11]
12	$[-y, -x, -z]$	[12]
13	$[y, -x, -z]$	[13]
14	$[-y, x, -z]$	[14]
15	$[-y, -x, z]$	[15]
16	$[y, x, z]$	[16]
17	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[17]
18	$\left[x+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[18]
19	$\left[\frac{1}{2}-x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[19]
20	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[20]
21	$\left[\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[22]
23	$\left[x+\frac{1}{2}, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[23]
24	$\left[x+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[24]
25	$\left[\frac{1}{2}-y, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[25]

continued ...

Table 15

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