MSG No. 139.538 $I4'/m'mm'$ [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	$\left[0, \frac{1}{2}, 0\right]$	[1,2,7,8,11,12,13,14]
2	$\left[\frac{1}{2}, 0, 0\right]$	[3,4,5,6,9,10,15,16]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[17,18,23,24,27,28,29,30]
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[19,20,21,22,25,26,31,32]

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, 0, 0]$	`[1,8,11,14]`
2	$[-x, 0, 0]$	`[2,7,12,13]`
3	$[0, x, 0]$	`[3,6,9,16]`

continued ...

Table 9

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,7]`

continued ...

Table 14

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