MSG No. 139.534 $I4'/mm'm$ [Type III, tetragonal]

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

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'/mm'm

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: mm'm'.

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

Table 4: Wyckoff site: 4d, site symmetry: -4'm'2

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

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

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m2'm'.`

No.	position	mapping
1	$[x, 0, 0]$	`[1,6,11,16]`
2	$[-x, 0, 0]$	`[2,5,12,15]`
3	$[0, x, 0]$	`[3,8,9,14]`

continued ...

Table 9

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

Table 10: Wyckoff site: `8j`, site symmetry: `m2'm'`.

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

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

No.	position	mapping
1	$\left[x, x+\frac{1}{2}, \frac{1}{4}\right]$	`[1,19]`
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	$\left[-x, \frac{1}{2}-x, \frac{3}{4}\right]$	`[5,23]`
6	$\left[x, x+\frac{1}{2}, \frac{3}{4}\right]$	`[6,24]`
7	$\left[\frac{1}{2}-x, -x, \frac{1}{4}\right]$	`[7,21]`
8	$\left[x+\frac{1}{2}, x, \frac{1}{4}\right]$	`[8,22]`
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	$\left[x+\frac{1}{2}, -x, \frac{3}{4}\right]$	`[13,32]`
14	$\left[\frac{1}{2}-x, x, \frac{3}{4}\right]$	`[14,31]`
15	$\left[-x, x+\frac{1}{2}, \frac{1}{4}\right]$	`[15,30]`
16	$\left[x, \frac{1}{2}-x, \frac{1}{4}\right]$	`[16,29]`

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,15]`

continued ...

Table 14

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

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	$[-x,\ -y,\ -z]$	[5]
6	$[x,\ y,\ -z]$	[6]
7	$[-y,\ -x,\ z]$	[7]
8	$[y,\ x,\ z]$	[8]
9	$[-y,\ x,\ z]$	[9]
10	$[y,\ -x,\ z]$	[10]
11	$[x,\ -y,\ -z]$	[11]
12	$[-x,\ y,\ -z]$	[12]
13	$[y,\ -x,\ -z]$	[13]
14	$[-y,\ x,\ -z]$	[14]
15	$[-x,\ y,\ z]$	[15]
16	$[x,\ -y,\ z]$	[16]
17	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[17]
18	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[21]
22	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[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	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[29]
30	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[31]
32	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[32]