MSG No. 141.558 $I4'_1/a'md'$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `-4m2`

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

Table 2: Wyckoff site: `4b`, site symmetry: `-4m2`

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

Table 3: Wyckoff site: `8c`, site symmetry: `.2'/m.`

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

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

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

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

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

Table 6: Wyckoff site: `16f`, site symmetry: `.2'.`

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

Table 7: Wyckoff site: `16g`, site symmetry: `..2`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	`[1,3]`
2	$\left[-x,\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	`[2,4]`
3	$\left[x,\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	`[5,8]`
4	$\left[-x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	`[6,7]`
5	$\left[-x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	`[9,12]`
6	$\left[x,\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	`[10,11]`
7	$\left[-x,\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	`[13,15]`
8	$\left[x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	`[14,16]`
9	$\left[x+\frac{1}{2},\ x+\frac{3}{4},\ \frac{3}{8}\right]$	`[17,19]`

continued ...

Table 7

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

Table 8: Wyckoff site: 16h, site symmetry: .m.

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

Table 9: Wyckoff site: 32i, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	[2]
3	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{3}{4}-z\right]$	[3]
4	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[4]
5	$\left[y+\frac{3}{4},\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[5]
6	$\left[\frac{1}{4}-y,\ x+\frac{1}{4},\ \frac{3}{4}-z\right]$	[6]
7	$[-x,\ y,\ z]$	[7]
8	$\left[x,\ \frac{1}{2}-y,\ z\right]$	[8]
9	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[9]
10	$\left[y+\frac{3}{4},\ \frac{3}{4}-x,\ z+\frac{1}{4}\right]$	[10]
11	$[x,\ -y,\ -z]$	[11]

continued ...

Table 9

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