MSG No. 141.559 $I4_1/a'm'd'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	`[1,7]`
2	$\left[-x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	`[2,5]`
3	$\left[x,\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	`[3,4]`
4	$\left[-x,\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	`[6,8]`
5	$\left[-x,\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	`[9,15]`
6	$\left[x,\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	`[10,13]`
7	$\left[-x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	`[11,12]`
8	$\left[x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	`[14,16]`
9	$\left[x+\frac{1}{2},\ x+\frac{3}{4},\ \frac{3}{8}\right]$	`[17,23]`

continued ...

Table 7

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

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

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

continued ...

Table 9

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