MSG No. 141.554 $I4_1'/am'd$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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	$[-x, 0, 0]$	[5,15]
6	$\left[x, \frac{1}{2}, 0\right]$	[6,16]
7	$\left[\frac{1}{4}, \frac{3}{4} - x, \frac{1}{4}\right]$	[7,29]
8	$\left[\frac{3}{4}, x + \frac{3}{4}, \frac{1}{4}\right]$	[8,30]
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	$\left[\frac{3}{4}, \frac{1}{4} - x, \frac{3}{4}\right]$	[13,23]
12	$\left[\frac{1}{4}, x + \frac{1}{4}, \frac{3}{4}\right]$	[14,24]
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	$\left[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}\right]$	[21,31]
16	$\left[x + \frac{1}{2}, 0, \frac{1}{2}\right]$	[22,32]

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	$\left[-x, \frac{3}{4} - x, \frac{1}{8}\right]$	[5,7]
4	$\left[x, x + \frac{3}{4}, \frac{1}{8}\right]$	[6,8]
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	$\left[x, \frac{1}{4} - x, \frac{7}{8}\right]$	[13,16]
8	$\left[-x, x + \frac{1}{4}, \frac{7}{8}\right]$	[14,15]
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	$\left[\frac{1}{2}-x,\ \frac{1}{4}-x,\ \frac{5}{8}\right]$	[21,23]
12	$\left[x+\frac{1}{2},\ x+\frac{1}{4},\ \frac{5}{8}\right]$	[22,24]
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	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{3}{8}\right]$	[29,32]
16	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ \frac{3}{8}\right]$	[30,31]

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

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

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	$[-x,\ -y,\ -z]$	[5]
6	$\left[x,\ y+\frac{1}{2},\ -z\right]$	[6]
7	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ z+\frac{1}{4}\right]$	[7]
8	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[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	$\left[y+\frac{3}{4},\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[13]
14	$\left[\frac{1}{4}-y,\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[14]
15	$\left[-x,\, y,\, z\right]$	[15]
16	$\left[x,\, \frac{1}{2}-y,\, z\right]$	[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	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[21]
22	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[22]
23	$\left[\frac{3}{4}-y,\, \frac{1}{4}-x,\, z+\frac{3}{4}\right]$	[23]
24	$\left[y+\frac{1}{4},\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[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	$\left[y+\frac{1}{4},\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[29]
30	$\left[\frac{3}{4}-y,\, x+\frac{3}{4},\, \frac{1}{4}-z\right]$	[30]
31	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[31]
32	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[32]