MSG No. 141.557 $I4_1/am'd'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 7

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

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

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

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	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	[4]
5	$[-x,\, -y,\, -z]$	[5]
6	$\left[y+\frac{3}{4},\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[6]
7	$\left[\frac{1}{4}-y,\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[7]
8	$\left[x,\, y+\frac{1}{2},\, -z\right]$	[8]
9	$[x,\, -y,\, -z]$	[9]
10	$\left[-x,\, y+\frac{1}{2},\, -z\right]$	[10]
11	$\left[y+\frac{3}{4},\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[11]

continued ...

Table 9

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