MSG No. 141.555 $I4_1'/amd'$ [Type III, tetragonal]

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

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

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

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	$[0,\ 0,\ 0]$	`[1,2,5,6]`
2	$\left[0,\ \frac{1}{2},\ 0\right]$	`[3,4,7,8]`
3	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[9,15,27,29]`
4	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[10,16,28,30]`
5	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[11,13,25,31]`
6	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[12,14,26,32]`
7	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[17,18,21,22]`
8	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[19,20,23,24]`

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

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

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

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

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

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

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	$\left[x,\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	`[2,10]`
3	$\left[-x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	`[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	$\left[-x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	`[6,14]`
7	$\left[x,\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	`[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	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{5}{8}\right]$	[18,26]
11	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ \frac{5}{8}\right]$	[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	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ \frac{3}{8}\right]$	[22,30]
15	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{3}{8}\right]$	[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	$[0,\ y,\ z]$	[1,6]
2	$[0,\ -y,\ -z]$	[2,5]
3	$\left[0,\ y+\frac{1}{2},\ -z\right]$	[3,8]
4	$\left[0,\ \frac{1}{2}-y,\ z\right]$	[4,7]
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	$\left[y+\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}-z\right]$	[11,13]
8	$\left[\frac{1}{4}-y,\ \frac{1}{4},\ \frac{3}{4}-z\right]$	[12,14]
9	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[17,22]
10	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[18,21]
11	$\left[\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[19,24]
12	$\left[\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[20,23]
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	$\left[y+\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}-z\right]$	[27,29]
16	$\left[\frac{3}{4}-y,\ \frac{3}{4},\ \frac{1}{4}-z\right]$	[28,30]

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

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

continued ...

Table 9

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