MSG No. 141.552 $I4_1/amd1'$ [Type II, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `-4m21'`

No.	position	mapping
1	$\left[0,\ \frac{3}{4},\ \frac{1}{8}\right]$	`[1,6,12,13,23,24,26,27,33,38,44,45,55,56,58,59]`
2	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{3}{8}\right]$	`[2,3,15,16,20,21,25,30,34,35,47,48,52,53,57,62]`
3	$\left[0,\ \frac{1}{4},\ \frac{7}{8}\right]$	`[4,5,9,14,18,19,31,32,36,37,41,46,50,51,63,64]`
4	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{5}{8}\right]$	`[7,8,10,11,17,22,28,29,39,40,42,43,49,54,60,61]`

Table 2: Wyckoff site: `4b`, site symmetry: `-4m21'`

No.	position	mapping
1	$\left[0,\ \frac{1}{4},\ \frac{3}{8}\right]$	`[1,6,7,8,10,11,12,13,33,38,39,40,42,43,44,45]`
2	$\left[0,\ \frac{3}{4},\ \frac{5}{8}\right]$	`[2,3,4,5,9,14,15,16,34,35,36,37,41,46,47,48]`
3	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{7}{8}\right]$	`[17,22,23,24,26,27,28,29,49,54,55,56,58,59,60,61]`
4	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{8}\right]$	`[18,19,20,21,25,30,31,32,50,51,52,53,57,62,63,64]`

Table 3: Wyckoff site: `8c`, site symmetry: `.2/m.1'`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,4,9,12,33,36,41,44]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[2,15,23,26,34,47,55,58]`
3	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[3,16,24,27,35,48,56,59]`
4	$\left[0,\ \frac{1}{2},\ 0\right]$	`[5,6,13,14,37,38,45,46]`
5	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[7,10,18,31,39,42,50,63]`
6	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[8,11,19,32,40,43,51,64]`
7	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[17,20,25,28,49,52,57,60]`
8	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[21,22,29,30,53,54,61,62]`

Table 4: Wyckoff site: `8d`, site symmetry: `.2/m.1'`

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[1,4,9,12,33,36,41,44]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}\right]$	`[2,15,23,26,34,47,55,58]`
3	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{3}{4}\right]$	`[3,16,24,27,35,48,56,59]`
4	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[5,6,13,14,37,38,45,46]`
5	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[7,10,18,31,39,42,50,63]`
6	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[8,11,19,32,40,43,51,64]`
7	$\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[17,20,25,28,49,52,57,60]`
8	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[21,22,29,30,53,54,61,62]`

Table 5: Wyckoff site: `8e`, site symmetry: `2mm.1'`

No.	position	mapping
1	$\left[0,\ \frac{1}{4},\ z\right]$	`[1,6,12,13,33,38,44,45]`
2	$\left[0,\ \frac{3}{4},\ z+\frac{1}{4}\right]$	`[2,3,15,16,34,35,47,48]`
3	$\left[0,\ \frac{3}{4},\ -z\right]$	`[4,5,9,14,36,37,41,46]`
4	$\left[0,\ \frac{1}{4},\ \frac{3}{4}-z\right]$	`[7,8,10,11,39,40,42,43]`
5	$\left[\frac{1}{2},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[17,22,28,29,49,54,60,61]`
6	$\left[\frac{1}{2},\ \frac{1}{4},\ z+\frac{3}{4}\right]$	`[18,19,31,32,50,51,63,64]`
7	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[20,21,25,30,52,53,57,62]`
8	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}-z\right]$	`[23,24,26,27,55,56,58,59]`

Table 6: Wyckoff site: `16f`, site symmetry: `.2.1'`

No.	position	mapping
1	$[x,\ 0,\ 0]$	`[1,4,33,36]`
2	$\left[\frac{1}{4},\ x+\frac{3}{4},\ \frac{1}{4}\right]$	`[2,23,34,55]`
3	$\left[\frac{3}{4},\ \frac{3}{4}-x,\ \frac{1}{4}\right]$	`[3,24,35,56]`
4	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[5,6,37,38]`
5	$\left[\frac{3}{4},\ x+\frac{1}{4},\ \frac{3}{4}\right]$	`[7,18,39,50]`
6	$\left[\frac{1}{4},\ \frac{1}{4}-x,\ \frac{3}{4}\right]$	`[8,19,40,51]`
7	$[-x,\ 0,\ 0]$	`[9,12,41,44]`
8	$\left[\frac{3}{4},\ \frac{1}{4}-x,\ \frac{3}{4}\right]$	`[10,31,42,63]`
9	$\left[\frac{1}{4},\ x+\frac{1}{4},\ \frac{3}{4}\right]$	`[11,32,43,64]`
10	$\left[x,\ \frac{1}{2},\ 0\right]$	`[13,14,45,46]`
11	$\left[\frac{1}{4},\ \frac{3}{4}-x,\ \frac{1}{4}\right]$	`[15,26,47,58]`
12	$\left[\frac{3}{4},\ x+\frac{3}{4},\ \frac{1}{4}\right]$	`[16,27,48,59]`
13	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[17,20,49,52]`
14	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$	`[21,22,53,54]`
15	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[25,28,57,60]`
16	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[29,30,61,62]`

Table 7: Wyckoff site: `16g`, site symmetry: `..21'`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	`[1,7,33,39]`
2	$\left[-x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	`[2,5,34,37]`
3	$\left[x,\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	`[3,4,35,36]`
4	$\left[-x,\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	`[6,8,38,40]`
5	$\left[-x,\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	`[9,15,41,47]`
6	$\left[x,\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	`[10,13,42,45]`
7	$\left[-x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	`[11,12,43,44]`
8	$\left[x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	`[14,16,46,48]`
9	$\left[x+\frac{1}{2},\ x+\frac{3}{4},\ \frac{3}{8}\right]$	`[17,23,49,55]`

continued ...

Table 7

No.	position	mapping
10	$\left[\frac{1}{2}-x,\, x+\frac{1}{4},\, \frac{5}{8}\right]$	[18,21,50,53]
11	$\left[x+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{5}{8}\right]$	[19,20,51,52]
12	$\left[\frac{1}{2}-x,\, \frac{3}{4}-x,\, \frac{3}{8}\right]$	[22,24,54,56]
13	$\left[\frac{1}{2}-x,\, \frac{1}{4}-x,\, \frac{5}{8}\right]$	[25,31,57,63]
14	$\left[x+\frac{1}{2},\, \frac{3}{4}-x,\, \frac{3}{8}\right]$	[26,29,58,61]
15	$\left[\frac{1}{2}-x,\, x+\frac{3}{4},\, \frac{3}{8}\right]$	[27,28,59,60]
16	$\left[x+\frac{1}{2},\, x+\frac{1}{4},\, \frac{5}{8}\right]$	[30,32,62,64]

Table 8: Wyckoff site: 16h, site symmetry: .m.1'

No.	position	mapping
1	$[0,\, y,\, z]$	[1,12,33,44]
2	$\left[\frac{1}{4}-y,\, \frac{3}{4},\, z+\frac{1}{4}\right]$	[2,15,34,47]
3	$\left[y+\frac{3}{4},\, \frac{3}{4},\, z+\frac{1}{4}\right]$	[3,16,35,48]
4	$[0,\, -y,\, -z]$	[4,9,36,41]
5	$\left[0,\, y+\frac{1}{2},\, -z\right]$	[5,14,37,46]
6	$\left[0,\, \frac{1}{2}-y,\, z\right]$	[6,13,38,45]
7	$\left[y+\frac{3}{4},\, \frac{1}{4},\, \frac{3}{4}-z\right]$	[7,10,39,42]
8	$\left[\frac{1}{4}-y,\, \frac{1}{4},\, \frac{3}{4}-z\right]$	[8,11,40,43]
9	$\left[\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[17,28,49,60]
10	$\left[\frac{3}{4}-y,\, \frac{1}{4},\, z+\frac{3}{4}\right]$	[18,31,50,63]
11	$\left[y+\frac{1}{4},\, \frac{1}{4},\, z+\frac{3}{4}\right]$	[19,32,51,64]
12	$\left[\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[20,25,52,57]
13	$\left[\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[21,30,53,62]
14	$\left[\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[22,29,54,61]
15	$\left[y+\frac{1}{4},\, \frac{3}{4},\, \frac{1}{4}-z\right]$	[23,26,55,58]
16	$\left[\frac{3}{4}-y,\, \frac{3}{4},\, \frac{1}{4}-z\right]$	[24,27,56,59]

Table 9: Wyckoff site: 32i, site symmetry: 11'

No.	position	mapping
1	$[x,\, y,\, z]$	[1,33]
2	$\left[\frac{1}{4}-y,\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[2,34]
3	$\left[y+\frac{3}{4},\, \frac{3}{4}-x,\, z+\frac{1}{4}\right]$	[3,35]
4	$[x,\, -y,\, -z]$	[4,36]
5	$\left[-x,\, y+\frac{1}{2},\, -z\right]$	[5,37]
6	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	[6,38]
7	$\left[y+\frac{3}{4},\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[7,39]
8	$\left[\frac{1}{4}-y,\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[8,40]
9	$[-x,\, -y,\, -z]$	[9,41]
10	$\left[y+\frac{3}{4},\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[10,42]
11	$\left[\frac{1}{4}-y,\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[11,43]

continued ...

Table 9

No.	position	mapping
12	$[-x,\, y,\, z]$	[12,44]
13	$\left[x,\, \frac{1}{2}-y,\, z\right]$	[13,45]
14	$\left[x,\, y+\frac{1}{2},\, -z\right]$	[14,46]
15	$\left[\frac{1}{4}-y,\, \frac{3}{4}-x,\, z+\frac{1}{4}\right]$	[15,47]
16	$\left[y+\frac{3}{4},\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[16,48]
17	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[17,49]
18	$\left[\frac{3}{4}-y,\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[18,50]
19	$\left[y+\frac{1}{4},\, \frac{1}{4}-x,\, z+\frac{3}{4}\right]$	[19,51]
20	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[20,52]
21	$\left[\frac{1}{2}-x,\, y,\, \frac{1}{2}-z\right]$	[21,53]
22	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[22,54]
23	$\left[y+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{4}-z\right]$	[23,55]
24	$\left[\frac{3}{4}-y,\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[24,56]
25	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[25,57]
26	$\left[y+\frac{1}{4},\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[26,58]
27	$\left[\frac{3}{4}-y,\, x+\frac{3}{4},\, \frac{1}{4}-z\right]$	[27,59]
28	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[28,60]
29	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[29,61]
30	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[30,62]
31	$\left[\frac{3}{4}-y,\, \frac{1}{4}-x,\, z+\frac{3}{4}\right]$	[31,63]
32	$\left[y+\frac{1}{4},\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[32,64]