MSG No. 140.542 $I4/mcm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `4221'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `-42m1'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `4/m..1'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `m.mm1'`

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

Table 5: Wyckoff site: `8e`, site symmetry: `..2/m1'`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,7,25,31,33,39,57,63]`
2	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[2,5,26,29,34,37,58,61]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 4..1'

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

Table 7: Wyckoff site: 8g, site symmetry: 2.mm1'

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

Table 8: Wyckoff site: 8h, site symmetry: m.2m1'

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, 0\right]$	[1,14,23,32,33,46,55,64]
2	$\left[\frac{1}{2} - x, x, 0\right]$	[2,11,21,28,34,43,53,60]
3	$\left[x + \frac{1}{2}, -x, 0\right]$	[3,10,20,29,35,42,52,61]
4	$\left[x, \frac{1}{2} - x, \frac{1}{2}\right]$	[4,13,19,26,36,45,51,58]
5	$\left[-x, x + \frac{1}{2}, \frac{1}{2}\right]$	[5,12,18,27,37,44,50,59]

continued ...

Table 8

No.	position	mapping
6	$\left[-x,\ \frac{1}{2}-x,\ 0\right]$	[6,9,24,31,38,41,56,63]
7	$\left[x+\frac{1}{2},\ x,\ \frac{1}{2}\right]$	[7,16,17,30,39,48,49,62]
8	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}\right]$	[8,15,22,25,40,47,54,57]

Table 9: Wyckoff site: 16i, site symmetry: ..21'

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

Table 10: Wyckoff site: 16j, site symmetry: .2.1'

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

continued ...

Table 10

No.	position	mapping
16	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{4}\right]$	`[29,30,61,62]`

Table 11: Wyckoff site: `16k`, site symmetry: `m..1'`

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

Table 12: Wyckoff site: `16l`, site symmetry: `..m1'`

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

Table 13: Wyckoff site: 32m, site symmetry: 11'

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