MSG No. 139.532 $I4/mmm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4/mmm1'

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

Table 2: Wyckoff site: 2b, site symmetry: 4/mmm1'

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

Table 3: Wyckoff site: 4c, site symmetry: mmm.1'

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

Table 4: Wyckoff site: 4d, site symmetry: -4m21'

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

Table 5: Wyckoff site: 4e, site symmetry: 4mm1'

No.	position	mapping
1	$[0, 0, z]$	[1,2,3,6,12,13,15,16,33,34,35,38,44,45,47,48]
2	$[0, 0, -z]$	[4,5,7,8,9,10,11,14,36,37,39,40,41,42,43,46]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: ..2/m1'

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

Table 7: Wyckoff site: 8g, site symmetry: 2mm.1'

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m2m.1'`

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

Table 10: Wyckoff site: `8j`, site symmetry: `m2m.1'`

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

Table 11: Wyckoff site: `16k`, site symmetry: `..21'`

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

Table 12: Wyckoff site: `16l`, 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	$[x,\ -y,\ 0]$	`[4,13,36,45]`
5	$[-x,\ y,\ 0]$	`[5,12,37,44]`
6	$[-x,\ -y,\ 0]$	`[6,9,38,41]`
7	$[y,\ x,\ 0]$	`[7,16,39,48]`
8	$[-y,\ -x,\ 0]$	`[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[20,29,52,61]`
13	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[21,28,53,60]`
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[22,25,54,57]`
15	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[23,32,55,64]`
16	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[24,31,56,63]`

Table 13: Wyckoff site: `16m`, site symmetry: `..m1'`

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

Table 14: Wyckoff site: `16n`, site symmetry: `.m.1'`

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,12,33,44]`

continued ...

Table 14

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

Table 15: Wyckoff site: `32o`, 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	$[x,\, -y,\, -z]$	`[4,36]`
5	$[-x,\, y,\, -z]$	`[5,37]`
6	$[-x,\, -y,\, z]$	`[6,38]`
7	$[y,\, x,\, -z]$	`[7,39]`
8	$[-y,\, -x,\, -z]$	`[8,40]`
9	$[-x,\, -y,\, -z]$	`[9,41]`
10	$[y,\, -x,\, -z]$	`[10,42]`
11	$[-y,\, x,\, -z]$	`[11,43]`
12	$[-x,\, y,\, z]$	`[12,44]`
13	$[x,\, -y,\, z]$	`[13,45]`
14	$[x,\, y,\, -z]$	`[14,46]`
15	$[-y,\, -x,\, z]$	`[15,47]`
16	$[y,\, x,\, z]$	`[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	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	`[20,52]`
21	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	`[21,53]`
22	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	`[22,54]`
23	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	`[23,55]`
24	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	`[24,56]`
25	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	`[25,57]`

continued ...

Table 15

No.	position	mapping
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	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[28,60]
29	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[29,61]
30	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[30,62]
31	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[31,63]
32	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[32,64]