MSG No. 140.545 $I4'/mcm'$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `4'22'`

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,11,21,31]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[2,10,22,30]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 4’..

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

Table 7: Wyckoff site: 8g, site symmetry: 2.m’m’

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

Table 8: Wyckoff site: 8h, site symmetry: m.2’m’

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, 0\right]$	[1,8,27,32]
2	$\left[x, \frac{1}{2} - x, \frac{1}{2}\right]$	[2,7,26,29]
3	$\left[-x, x + \frac{1}{2}, \frac{1}{2}\right]$	[3,6,25,30]
4	$\left[-x, \frac{1}{2} - x, 0\right]$	[4,5,28,31]
5	$\left[\frac{1}{2} - x, x, 0\right]$	[9,14,19,22]

continued ...

Table 8

No.	position	mapping
6	$\left[x+\frac{1}{2},\ -x,\ 0\right]$	[10,13,18,23]
7	$\left[x+\frac{1}{2},\ x,\ \frac{1}{2}\right]$	[11,16,17,24]
8	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}\right]$	[12,15,20,21]

Table 9: Wyckoff site: 16i, site symmetry: ..2'

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

Table 10: Wyckoff site: 16j, site symmetry: .2.

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

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{2}, x+\frac{1}{2}, \frac{1}{4}\right]$	[30,32]

Table 11: Wyckoff site: 16k, site symmetry: m..

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

Table 12: Wyckoff site: 16l, site symmetry: ..m'

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

Table 13: Wyckoff site: `32m`, site symmetry: `1`

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