MSG No. 140.544 $I4'/mc'm$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `4'2'2`

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: `-4'2'm`

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,3,21,23]`
2	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[2,4,22,24]`

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, x + \frac{1}{2}, 0\right]$	[1,6,19,24]
2	$\left[-x, \frac{1}{2} - x, 0\right]$	[2,5,20,23]
3	$\left[x + \frac{1}{2}, x, \frac{1}{2}\right]$	[3,8,17,22]
4	$\left[\frac{1}{2} - x, -x, \frac{1}{2}\right]$	[4,7,18,21]
5	$\left[\frac{1}{2} - x, x, 0\right]$	[9,14,28,31]

continued ...

Table 8

No.	position	mapping
6	$\left[x+\frac{1}{2},\ -x,\ 0\right]$	[10,13,27,32]
7	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[11,16,26,29]
8	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[12,15,25,30]

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

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

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

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

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{4}\right]$	[24,30]

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

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

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

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

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

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