MSG No. 132.458 P_I4_2/mcm [Type IV, tetragonal]

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

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

Table 2: Wyckoff site: 4b, site symmetry: -42m

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,15,23,25]
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[2,13,21,26]

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[x, x, 0]$	[1,7,14,16]
2	$\left[-x, x, \frac{1}{2}\right]$	[2,5,11,12]
3	$\left[x, -x, \frac{1}{2}\right]$	[3,4,10,13]
4	$[-x, -x, 0]$	[6,8,9,15]
5	$\left[x+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}\right]$	[17,23,30,32]

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2}-x,\, x+\frac{1}{2},\, 0\right]$	[18,21,27,28]
7	$\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, 0\right]$	[19,20,26,29]
8	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[22,24,25,31]

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

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

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

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

continued …

Table 10

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

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

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

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

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

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

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