MSG No. 131.445 P_C4_2/mmc [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: mmm.

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

Table 2: Wyckoff site: 4b, site symmetry: -4m2

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: -4'm2'

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

Table 5: Wyckoff site: 8e, site symmetry: 2.22

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,8,22,23]
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[2,4,19,21]

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	[1,6,12,13]
2	$\left[\frac{1}{2}, 0, z + \frac{1}{2}\right]$	[2,3,15,16]
3	$\left[0, \frac{1}{2}, -z\right]$	[4,5,9,14]
4	$\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$	[7,8,10,11]
5	$\left[\frac{1}{2}, 0, z\right]$	[17,22,28,29]

Table 8

No.	position	mapping
6	$\left[0, \frac{1}{2}, z + \frac{1}{2}\right]$	[18,19,31,32]
7	$\left[\frac{1}{2}, 0, -z\right]$	[20,21,25,30]
8	$\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$	[23,24,26,27]

Table 9: Wyckoff site: `8i`, site symmetry: `mm2`.

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

Table 10: Wyckoff site: `8j`, site symmetry: `mm2`.

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

Table 11: Wyckoff site: `16k`, site symmetry: `2'..`.

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

continued ...

Table 11

No.	position	mapping
9	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	[9,30]
10	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z\right]$	[10,27]
11	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	[11,26]
12	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	[12,29]
13	$\left[\frac{3}{4}, \frac{3}{4}, z\right]$	[13,28]
14	$\left[\frac{3}{4}, \frac{1}{4}, -z\right]$	[14,25]
15	$\left[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}\right]$	[15,32]
16	$\left[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}\right]$	[16,31]

Table 12: Wyckoff site: `16l`, site symmetry: `..2`

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

Table 13: Wyckoff site: `16m`, 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	$\left[x, \frac{1}{2} - x, \frac{3}{4}\right]$	[4,19]
5	$\left[-x, x + \frac{1}{2}, \frac{3}{4}\right]$	[5,18]
6	$\left[-x, \frac{1}{2} - x, \frac{1}{4}\right]$	[6,24]
7	$\left[x + \frac{1}{2}, x, \frac{1}{4}\right]$	[7,17]
8	$\left[\frac{1}{2} - x, -x, \frac{1}{4}\right]$	[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]

continued ...

Table 13

No.	position	mapping
11	$\left[\frac{1}{2} - x,\, x,\, \frac{1}{4}\right]$	[11,28]
12	$\left[-x,\, x + \frac{1}{2},\, \frac{1}{4}\right]$	[12,27]
13	$\left[x,\, \frac{1}{2} - x,\, \frac{1}{4}\right]$	[13,26]
14	$\left[x,\, x + \frac{1}{2},\, \frac{3}{4}\right]$	[14,32]
15	$\left[\frac{1}{2} - x,\, -x,\, \frac{3}{4}\right]$	[15,25]
16	$\left[x + \frac{1}{2},\, x,\, \frac{3}{4}\right]$	[16,30]

Table 14: Wyckoff site: 16n, 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	$[x,\, -y,\, 0]$	[4,13]
5	$[-x,\, y,\, 0]$	[5,12]
6	$[-x,\, -y,\, 0]$	[6,9]
7	$\left[y,\, x,\, \frac{1}{2}\right]$	[7,16]
8	$\left[-y,\, -x,\, \frac{1}{2}\right]$	[8,15]
9	$\left[x + \frac{1}{2},\, y + \frac{1}{2},\, 0\right]$	[17,30]
10	$\left[\frac{1}{2} - y,\, x + \frac{1}{2},\, \frac{1}{2}\right]$	[18,27]
11	$\left[y + \frac{1}{2},\, \frac{1}{2} - x,\, \frac{1}{2}\right]$	[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	$\left[\frac{1}{2} - x,\, \frac{1}{2} - y,\, 0\right]$	[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 15: Wyckoff site: 16o, site symmetry: .m.

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

continued …

Table 15

No.	position	mapping
13	$\left[\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[21,30]
14	$\left[\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[22,29]
15	$\left[y+\frac{1}{2},\, \frac{1}{2},\, \frac{1}{2}-z\right]$	[23,26]
16	$\left[\frac{1}{2}-y,\, \frac{1}{2},\, \frac{1}{2}-z\right]$	[24,27]

Table 16: Wyckoff site: 32p, 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	$[x,\, -y,\, -z]$	[4]
5	$[-x,\, y,\, -z]$	[5]
6	$[-x,\, -y,\, z]$	[6]
7	$\left[y,\, x,\, \frac{1}{2}-z\right]$	[7]
8	$\left[-y,\, -x,\, \frac{1}{2}-z\right]$	[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	$[-x,\, y,\, z]$	[12]
13	$[x,\, -y,\, z]$	[13]
14	$[x,\, y,\, -z]$	[14]
15	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[15]
16	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[16]
17	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z\right]$	[17]
18	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[18]
19	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z\right]$	[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	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[25]
26	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[26]
27	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[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	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[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]