MSG No. 131.446 P_I4_2/mmc [Type IV, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, 0, 0]$	`[1,4,13,14]`
2	$\left[0, x, \frac{1}{2}\right]$	`[2,7,11,16]`
3	$\left[0, -x, \frac{1}{2}\right]$	`[3,8,10,15]`

continued ...

Table 9

No.	position	mapping
4	$[-x,\ 0,\ 0]$	`[5,6,9,12]`
5	$[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}]$	`[17,20,29,30]`
6	$[\frac{1}{2},\ x+\frac{1}{2},\ 0]$	`[18,23,27,32]`
7	$[\frac{1}{2},\ \frac{1}{2}-x,\ 0]$	`[19,24,26,31]`
8	$[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}]$	`[21,22,25,28]`

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

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

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

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

Table 12: Wyckoff site: `16l`, 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	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[20,29]`
13	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[21,28]`
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[22,25]`
15	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	`[23,32]`
16	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ 0\right]$	`[24,31]`

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2},\ y,\ z\right]$	`[1,12]`

continued ...

Table 14

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

Table 15: Wyckoff site: 32o, 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	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[20]
21	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[22]
23	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	[23]
24	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ -z\right]$	[24]
25	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[25]

continued ...

Table 15

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