MSG No. 223.107 $Pm\bar{3}n'$ [Type III, cubic]

Table 1: Wyckoff site: `2a`, site symmetry: `m-3.`

No.	position	mapping
1	[0, 0, 0]	`[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]`

Table 2: Wyckoff site: `6b`, site symmetry: `mmm..`

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[1,2,3,4,13,14,15,16]`
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[5,8,10,12,17,20,22,24]`
3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[6,7,9,11,18,19,21,23]`
4	$\left[\frac{1}{2}, 0, 0\right]$	`[25,26,33,34,37,38,45,46]`
5	$\left[0, 0, \frac{1}{2}\right]$	`[27,28,35,36,39,40,47,48]`
6	$\left[0, \frac{1}{2}, 0\right]$	`[29,30,31,32,41,42,43,44]`

Table 3: Wyckoff site: `6c`, site symmetry: `-4'm.2'`

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[1,2,15,16,33,34,37,38]`
2	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	`[3,4,13,14,25,26,45,46]`
3	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	`[5,12,20,22,30,32,41,43]`
4	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[6,9,19,23,27,36,40,47]`
5	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	`[7,11,18,21,28,35,39,48]`
6	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	`[8,10,17,24,29,31,42,44]`

Table 4: Wyckoff site: `6d`, site symmetry: `-4'm.2'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	`[1,2,15,16,33,34,37,38]`
2	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	`[3,4,13,14,25,26,45,46]`
3	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	`[5,12,20,22,30,32,41,43]`
4	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[6,9,19,23,27,36,40,47]`
5	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[7,11,18,21,28,35,39,48]`
6	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	`[8,10,17,24,29,31,42,44]`

Table 5: Wyckoff site: `8e`, site symmetry: `.32'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,5,6,32,34,36]`
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[2,10,11,28,29,33]`
3	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[3,7,12,25,30,35]`
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[4,8,9,26,27,31]`
5	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[13,17,18,44,46,48]`
6	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[14,22,23,40,41,45]`
7	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[15,19,24,37,42,47]`
8	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[16,20,21,38,39,43]`

Table 6: Wyckoff site: `12f`, site symmetry: `2mm..`

No.	position	mapping
1	$[x, 0, 0]$	`[1,2,15,16]`
2	$[-x, 0, 0]$	`[3,4,13,14]`
3	$[0, x, 0]$	`[5,12,20,22]`
4	$[0, 0, x]$	`[6,9,19,23]`
5	$[0, 0, -x]$	`[7,11,18,21]`
6	$[0, -x, 0]$	`[8,10,17,24]`
7	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[25,26,45,46]`
8	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x\right]$	`[27,36,40,47]`
9	$\left[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}\right]$	`[28,35,39,48]`
10	$\left[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}\right]$	`[29,31,42,44]`
11	$\left[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}\right]$	`[30,32,41,43]`
12	$\left[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}\right]$	`[33,34,37,38]`

Table 7: Wyckoff site: `12g`, site symmetry: `2mm..`

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	`[1,2,15,16]`
2	$\left[-x, 0, \frac{1}{2}\right]$	`[3,4,13,14]`
3	$\left[\frac{1}{2}, x, 0\right]$	`[5,12,20,22]`
4	$\left[0, \frac{1}{2}, x\right]$	`[6,9,19,23]`
5	$\left[0, \frac{1}{2}, -x\right]$	`[7,11,18,21]`
6	$\left[\frac{1}{2}, -x, 0\right]$	`[8,10,17,24]`
7	$\left[x + \frac{1}{2}, 0, \frac{1}{2}\right]$	`[25,26,45,46]`
8	$\left[0, \frac{1}{2}, \frac{1}{2} - x\right]$	`[27,36,40,47]`
9	$\left[0, \frac{1}{2}, x + \frac{1}{2}\right]$	`[28,35,39,48]`
10	$\left[\frac{1}{2}, x + \frac{1}{2}, 0\right]$	`[29,31,42,44]`
11	$\left[\frac{1}{2}, \frac{1}{2} - x, 0\right]$	`[30,32,41,43]`
12	$\left[\frac{1}{2} - x, 0, \frac{1}{2}\right]$	`[33,34,37,38]`

Table 8: Wyckoff site: `12h`, site symmetry: `2mm..`

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ 0\right]$	`[1,2,15,16]`
2	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[3,4,13,14]`
3	$\left[0,\ x,\ \frac{1}{2}\right]$	`[5,12,20,22]`
4	$\left[\frac{1}{2},\ 0,\ x\right]$	`[6,9,19,23]`
5	$\left[\frac{1}{2},\ 0,\ -x\right]$	`[7,11,18,21]`
6	$\left[0,\ -x,\ \frac{1}{2}\right]$	`[8,10,17,24]`
7	$\left[x+\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[25,26,45,46]`
8	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-x\right]$	`[27,36,40,47]`
9	$\left[\frac{1}{2},\ 0,\ x+\frac{1}{2}\right]$	`[28,35,39,48]`
10	$\left[0,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[29,31,42,44]`
11	$\left[0,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[30,32,41,43]`
12	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ 0\right]$	`[33,34,37,38]`

Table 9: Wyckoff site: `16i`, site symmetry: `.3.`

No.	position	mapping
1	$[x,\ x,\ x]$	`[1,5,6]`
2	$[x,\ -x,\ -x]$	`[2,10,11]`
3	$[-x,\ x,\ -x]$	`[3,7,12]`
4	$[-x,\ -x,\ x]$	`[4,8,9]`
5	$[-x,\ -x,\ -x]$	`[13,17,18]`
6	$[-x,\ x,\ x]$	`[14,22,23]`
7	$[x,\ -x,\ x]$	`[15,19,24]`
8	$[x,\ x,\ -x]$	`[16,20,21]`
9	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	`[25,30,35]`
10	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$	`[26,27,31]`
11	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	`[28,29,33]`
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	`[32,34,36]`
13	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$	`[37,42,47]`
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	`[38,39,43]`
15	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	`[40,41,45]`
16	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	`[44,46,48]`

Table 10: Wyckoff site: `24j`, site symmetry: `..2'`

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ y+\frac{1}{2}\right]$	`[1,33]`
2	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}-y\right]$	`[2,34]`
3	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	`[3,26]`
4	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	`[4,25]`
5	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y\right]$	`[5,30]`

continued ...

Table 10

No.	position	mapping
6	$\left[y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[6,27]
7	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[7,28]
8	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ y\right]$	[8,29]
9	$\left[-y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[9,36]
10	$\left[y+\frac{1}{2},\ \frac{3}{4},\ -y\right]$	[10,31]
11	$\left[y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[11,35]
12	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ -y\right]$	[12,32]
13	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}-y\right]$	[13,45]
14	$\left[\frac{3}{4},\ y,\ y+\frac{1}{2}\right]$	[14,46]
15	$\left[\frac{1}{4},\ -y,\ y+\frac{1}{2}\right]$	[15,38]
16	$\left[\frac{1}{4},\ y,\ \frac{1}{2}-y\right]$	[16,37]
17	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ -y\right]$	[17,42]
18	$\left[-y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[18,39]
19	$\left[y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[19,40]
20	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[20,41]
21	$\left[y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[21,48]
22	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ y\right]$	[22,43]
23	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[23,47]
24	$\left[y+\frac{1}{2},\ \frac{3}{4},\ y\right]$	[24,44]

Table 11: Wyckoff site: 24k, site symmetry: m..

No.	position	mapping
1	$[0,\ y,\ z]$	[1,14]
2	$[0,\ -y,\ -z]$	[2,13]
3	$[0,\ y,\ -z]$	[3,16]
4	$[0,\ -y,\ z]$	[4,15]
5	$[z,\ 0,\ y]$	[5,24]
6	$[y,\ z,\ 0]$	[6,21]
7	$[-y,\ z,\ 0]$	[7,23]
8	$[-z,\ 0,\ y]$	[8,22]
9	$[-y,\ -z,\ 0]$	[9,18]
10	$[z,\ 0,\ -y]$	[10,20]
11	$[y,\ -z,\ 0]$	[11,19]
12	$[-z,\ 0,\ -y]$	[12,17]
13	$\left[\frac{1}{2},\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	[25,38]
14	$\left[\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	[26,37]
15	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[27,48]
16	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[28,47]
17	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[29,43]
18	$\left[y+\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[30,44]
19	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[31,41]
20	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[32,42]
21	$\left[\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[33,46]

continued ...

Table 11

No.	position	mapping
22	$\left[\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[34,45]
23	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[35,40]
24	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[36,39]

Table 12: Wyckoff site: 48l, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[x,\ -y,\ -z]$	[2]
3	$[-x,\ y,\ -z]$	[3]
4	$[-x,\ -y,\ z]$	[4]
5	$[z,\ x,\ y]$	[5]
6	$[y,\ z,\ x]$	[6]
7	$[-y,\ z,\ -x]$	[7]
8	$[-z,\ -x,\ y]$	[8]
9	$[-y,\ -z,\ x]$	[9]
10	$[z,\ -x,\ -y]$	[10]
11	$[y,\ -z,\ -x]$	[11]
12	$[-z,\ x,\ -y]$	[12]
13	$[-x,\ -y,\ -z]$	[13]
14	$[-x,\ y,\ z]$	[14]
15	$[x,\ -y,\ z]$	[15]
16	$[x,\ y,\ -z]$	[16]
17	$[-z,\ -x,\ -y]$	[17]
18	$[-y,\ -z,\ -x]$	[18]
19	$[y,\ -z,\ x]$	[19]
20	$[z,\ x,\ -y]$	[20]
21	$[y,\ z,\ -x]$	[21]
22	$[-z,\ x,\ y]$	[22]
23	$[-y,\ z,\ x]$	[23]
24	$[z,\ -x,\ y]$	[24]
25	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	[25]
26	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	[26]
27	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-x\right]$	[27]
28	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[28]
29	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[29]
30	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[30]
31	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[31]
32	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[32]
33	$\left[\frac{1}{2}-x,\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[33]
34	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[34]
35	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ x+\frac{1}{2}\right]$	[35]
36	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[36]
37	$\left[\frac{1}{2}-x,\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	[37]

continued ...

Table 12

No.	position	mapping
38	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	[38]
39	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ x+\frac{1}{2}\right]$	[39]
40	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[40]
41	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[41]
42	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[42]
43	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[43]
44	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[44]
45	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[45]
46	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[46]
47	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ \frac{1}{2}-x\right]$	[47]
48	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[48]