MSG No. 223.106 $Pm'\bar{3}'n$ [Type III, cubic]

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

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

Table 2: Wyckoff site: `6b`, site symmetry: `m'm'm'..`

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

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

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

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

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

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	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[13,18,23,39,43,48]`
6	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[14,15,19,40,44,45]`
7	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[16,17,21,38,46,47]`
8	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[20,22,24,37,41,42]`

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

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

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

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

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

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

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	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$	`[13,18,23]`
6	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	`[14,15,19]`
7	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	`[16,17,21]`
8	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	`[20,22,24]`
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	$[-x,\ -x,\ -x]$	`[37,41,42]`
14	$[-x,\ x,\ x]$	`[38,46,47]`
15	$[x,\ -x,\ x]$	`[39,43,48]`
16	$[x,\ x,\ -x]$	`[40,44,45]`

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	$\left[\frac{1}{4},\ y,\ \frac{1}{2}-y\right]$	[13,40]
14	$\left[\frac{1}{4},\ -y,\ y+\frac{1}{2}\right]$	[14,39]
15	$\left[-y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[15,42]
16	$\left[y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[16,43]
17	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[17,44]
18	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ -y\right]$	[18,41]
19	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ y\right]$	[19,46]
20	$\left[y+\frac{1}{2},\ \frac{3}{4},\ y\right]$	[20,48]
21	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}-y\right]$	[21,37]
22	$\left[\frac{3}{4},\ y,\ y+\frac{1}{2}\right]$	[22,38]
23	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[23,47]
24	$\left[y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[24,45]

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

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

continued ...

Table 11

No.	position	mapping
22	$\left[\frac{1}{2},\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[22,33]
23	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[23,28]
24	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[24,27]

Table 12: Wyckoff site: 481, 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	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, \frac{1}{2}-y\right]$	[13]
14	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, y+\frac{1}{2}\right]$	[14]
15	$\left[\frac{1}{2}-z,\, \frac{1}{2}-y,\, x+\frac{1}{2}\right]$	[15]
16	$\left[z+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[16]
17	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[17]
18	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[18]
19	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[19]
20	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[20]
21	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[21]
22	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[22]
23	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[23]
24	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[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	$[-x,\, -y,\, -z]$	[37]

continued ...

Table 12

No.	position	mapping
38	$[-x,\ y,\ z]$	[38]
39	$[x,\ -y,\ z]$	[39]
40	$[x,\ y,\ -z]$	[40]
41	$[-z,\ -x,\ -y]$	[41]
42	$[-y,\ -z,\ -x]$	[42]
43	$[y,\ -z,\ x]$	[43]
44	$[z,\ x,\ -y]$	[44]
45	$[y,\ z,\ -x]$	[45]
46	$[-z,\ x,\ y]$	[46]
47	$[-y,\ z,\ x]$	[47]
48	$[z,\ -x,\ y]$	[48]