MSG No. 223.104 $Pm\bar{3}n$ [Type I, cubic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ y+\frac{1}{2}\right]$	`[1,13]`
2	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	`[2,10]`
3	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	`[3,9]`
4	$\left[y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	`[4,18]`
5	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	`[5,19]`

continued ...

Table 10

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

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

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

continued ...

Table 11

No.	position	mapping
22	$[z,\ 0,\ -y]$	`[22,44]`
23	$[y,\ -z,\ 0]$	`[23,43]`
24	$[-z,\ 0,\ -y]$	`[24,41]`

Table 12: Wyckoff site: `481`, site symmetry: `1`

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

continued ...

Table 12

No.	position	mapping
38	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[38]
39	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[39]
40	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[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]