MSG No. 200.17 $P_Im\bar{3}$ [Type IV, 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	$\left[\frac{1}{2}, 0, 0\right]$	[25,26,27,28,37,38,39,40]
5	$\left[0, \frac{1}{2}, 0\right]$	[29,32,34,36,41,44,46,48]
6	$\left[0, 0, \frac{1}{2}\right]$	[30,31,33,35,42,43,45,47]

Table 3: Wyckoff site: 8c, site symmetry: .-3'.

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

Table 4: Wyckoff site: 12d, 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	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[25,26,39,40]
8	$\left[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}\right]$	[27,28,37,38]
9	$\left[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}\right]$	[29,36,44,46]

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{2}, \frac{1}{2}, x+\frac{1}{2}\right]$	[30,33,43,47]
11	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-x\right]$	[31,35,42,45]
12	$\left[\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	[32,34,41,48]

Table 5: Wyckoff site: 12e, 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	$\left[x+\frac{1}{2}, \frac{1}{2}, 0\right]$	[25,26,39,40]
8	$\left[\frac{1}{2}-x, \frac{1}{2}, 0\right]$	[27,28,37,38]
9	$\left[0, x+\frac{1}{2}, \frac{1}{2}\right]$	[29,36,44,46]
10	$\left[\frac{1}{2}, 0, x+\frac{1}{2}\right]$	[30,33,43,47]
11	$\left[\frac{1}{2}, 0, \frac{1}{2}-x\right]$	[31,35,42,45]
12	$\left[0, \frac{1}{2}-x, \frac{1}{2}\right]$	[32,34,41,48]

Table 6: Wyckoff site: 16f, 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	$\left[x+\frac{1}{2}, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[25,29,30]
10	$\left[x+\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[26,34,35]
11	$\left[\frac{1}{2}-x, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[27,31,36]
12	$\left[\frac{1}{2}-x, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[28,32,33]
13	$\left[\frac{1}{2}-x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[37,41,42]
14	$\left[\frac{1}{2}-x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[38,46,47]
15	$\left[x+\frac{1}{2}, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[39,43,48]
16	$\left[x+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[40,44,45]

Table 7: Wyckoff site: `24g`, 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	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[25,38]`
14	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	`[26,37]`
15	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[27,40]`
16	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[28,39]`
17	$\left[z+\frac{1}{2},\ \frac{1}{2},\ y+\frac{1}{2}\right]$	`[29,48]`
18	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{2}\right]$	`[30,45]`
19	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ \frac{1}{2}\right]$	`[31,47]`
20	$\left[\frac{1}{2}-z,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	`[32,46]`
21	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ \frac{1}{2}\right]$	`[33,42]`
22	$\left[z+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-y\right]$	`[34,44]`
23	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}\right]$	`[35,43]`
24	$\left[\frac{1}{2}-z,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	`[36,41]`

Table 8: Wyckoff site: `48h`, 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]`

continued ...

Table 8

No.	position	mapping
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	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[25]
26	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[26]
27	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27]
28	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[28]
29	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[29]
30	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[30]
31	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[31]
32	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$	[32]
33	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$	[33]
34	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[34]
35	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[35]
36	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[36]
37	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[37]
38	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[38]
39	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[39]
40	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[40]
41	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[41]
42	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[42]
43	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$	[43]
44	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[44]
45	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[45]
46	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[46]
47	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[47]
48	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$	[48]