MSG No. 221.94 $Pm'\bar{3}'m$ [Type III, cubic]

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

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, 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: `1b`, site symmetry: `m'-3'm`

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24, 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 3: Wyckoff site: `3c`, site symmetry: `4'/m'm'.m`

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

Table 4: Wyckoff site: `3d`, site symmetry: `4'/m'm'.m`

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

Table 5: Wyckoff site: `6e`, site symmetry: `4'm'.m`

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

Table 6: Wyckoff site: `6f`, site symmetry: `4'm'.m`

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

Table 7: Wyckoff site: `8g`, site symmetry: `.3m`

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

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	$\left[-x, 0, \frac{1}{2}\right]$	[13,14,33,34]
8	$\left[0, \frac{1}{2}, x\right]$	[15,24,28,35]
9	$\left[0, \frac{1}{2}, -x\right]$	[16,23,27,36]
10	$\left[\frac{1}{2}, -x, 0\right]$	[17,19,30,32]
11	$\left[\frac{1}{2}, x, 0\right]$	[18,20,29,31]
12	$\left[x, 0, \frac{1}{2}\right]$	[21,22,25,26]

Table 9: Wyckoff site: `12i`, site symmetry: `m'.2'm`

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

Table 10: Wyckoff site: `12j`, site symmetry: `m'.2'm`

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

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]`

continued …

Table 11

No.	position	mapping
10	$[z, 0, -y]$	[10,44]
11	$[y, -z, 0]$	[11,43]
12	$[-z, 0, -y]$	[12,41]
13	$[0, z, -y]$	[13,26]
14	$[0, -z, y]$	[14,25]
15	$[-z, -y, 0]$	[15,36]
16	$[z, -y, 0]$	[16,35]
17	$[y, 0, -z]$	[17,31]
18	$[-y, 0, -z]$	[18,32]
19	$[-y, 0, z]$	[19,29]
20	$[y, 0, z]$	[20,30]
21	$[0, -z, -y]$	[21,34]
22	$[0, z, y]$	[22,33]
23	$[-z, y, 0]$	[23,28]
24	$[z, y, 0]$	[24,27]

Table 12: Wyckoff site: 241, site symmetry: m'..

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

Table 13: Wyckoff site: `24m`, site symmetry: `..m`

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

Table 14: Wyckoff site: `48n`, 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	$[-x,\, z,\, -y]$	[13]
14	$[-x,\, -z,\, y]$	[14]
15	$[-z,\, -y,\, x]$	[15]

continued …

Table 14

No.	position	mapping
16	$[z, -y, -x]$	[16]
17	$[y, -x, -z]$	[17]
18	$[-y, x, -z]$	[18]
19	$[-y, -x, z]$	[19]
20	$[y, x, z]$	[20]
21	$[x, -z, -y]$	[21]
22	$[x, z, y]$	[22]
23	$[-z, y, -x]$	[23]
24	$[z, y, x]$	[24]
25	$[x, -z, y]$	[25]
26	$[x, z, -y]$	[26]
27	$[z, y, -x]$	[27]
28	$[-z, y, x]$	[28]
29	$[-y, x, z]$	[29]
30	$[y, -x, z]$	[30]
31	$[y, x, -z]$	[31]
32	$[-y, -x, -z]$	[32]
33	$[-x, z, y]$	[33]
34	$[-x, -z, -y]$	[34]
35	$[z, -y, x]$	[35]
36	$[-z, -y, -x]$	[36]
37	$[-x, -y, -z]$	[37]
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]