MSG No. 221.96 $Pm'\bar{3}'m'$ [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	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,3,8,9,10,13,14,25,26,27,32,33,34,37,38]
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[4,5,15,16,18,19,21,23,28,29,39,40,42,43,45,47]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[6,7,11,12,17,20,22,24,30,31,35,36,41,44,46,48]

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, \frac{1}{2}, 0\right]$	`[1,8,33,34]`
2	$\left[x, 0, \frac{1}{2}\right]$	`[2,3,37,38]`
3	$\left[0, \frac{1}{2}, -x\right]$	`[4,16,29,39]`
4	$\left[0, \frac{1}{2}, x\right]$	`[5,15,28,40]`
5	$\left[\frac{1}{2}, x, 0\right]$	`[6,11,31,36]`
6	$\left[\frac{1}{2}, -x, 0\right]$	`[7,12,30,35]`
7	$\left[-x, \frac{1}{2}, 0\right]$	`[9,10,25,32]`
8	$\left[-x, 0, \frac{1}{2}\right]$	`[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: `12i`, site symmetry: `m'.2m'`

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,32]`
2	$[0,\ -z,\ y]$	`[2,27]`
3	$[0,\ z,\ -y]$	`[3,26]`
4	$[z,\ y,\ 0]$	`[4,40]`
5	$[-z,\ y,\ 0]$	`[5,39]`
6	$[-y,\ 0,\ z]$	`[6,35]`
7	$[y,\ 0,\ z]$	`[7,36]`
8	$[0,\ -y,\ -z]$	`[8,25]`
9	$[0,\ y,\ -z]$	`[9,34]`

continued ...

Table 11

No.	position	mapping
10	$[0, -y, z]$	[10,33]
11	$[y, 0, -z]$	[11,30]
12	$[-y, 0, -z]$	[12,31]
13	$[0, z, y]$	[13,38]
14	$[0, -z, -y]$	[14,37]
15	$[z, -y, 0]$	[15,29]
16	$[-z, -y, 0]$	[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]
22	$[z, 0, -y]$	[22,44]
23	$[y, -z, 0]$	[23,43]
24	$[-z, 0, -y]$	[24,41]

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

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

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

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

Table 14: Wyckoff site: 48n, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -z, y]$	[2]
3	$[x, z, -y]$	[3]
4	$[z, y, -x]$	[4]
5	$[-z, y, x]$	[5]
6	$[-y, x, z]$	[6]
7	$[y, -x, z]$	[7]
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]
10	$[-x, -y, z]$	[10]
11	$[y, x, -z]$	[11]
12	$[-y, -x, -z]$	[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	$[z, x, y]$	[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	$[-x, z, -y]$	[26]
27	$[-x, -z, y]$	[27]
28	$[-z, -y, x]$	[28]
29	$[z, -y, -x]$	[29]
30	$[y, -x, -z]$	[30]
31	$[-y, x, -z]$	[31]
32	$[-x, y, z]$	[32]
33	$[x, -y, z]$	[33]
34	$[x, y, -z]$	[34]
35	$[-y, -x, z]$	[35]
36	$[y, x, z]$	[36]
37	$[x, -z, -y]$	[37]
38	$[x, z, y]$	[38]
39	$[-z, y, -x]$	[39]
40	$[z, y, x]$	[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]