MSG No. 221.95 $Pm\bar{3}m'$ [Type III, cubic]

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

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-3m'`

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'/mm.m'`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 11: Wyckoff site: `24k`, 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]`

continued ...

Table 11

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

Table 12: Wyckoff site: 24l, site symmetry: m..

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

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

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

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	$[-x, -y, -z]$	[13]
14	$[-x, y, z]$	[14]
15	$[x, -y, z]$	[15]

continued ...

Table 14

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	$[x, -z, y]$	[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	$[-x, z, -y]$	[37]
38	$[-x, -z, y]$	[38]
39	$[-z, -y, x]$	[39]
40	$[z, -y, -x]$	[40]
41	$[y, -x, -z]$	[41]
42	$[-y, x, -z]$	[42]
43	$[-y, -x, z]$	[43]
44	$[y, x, z]$	[44]
45	$[x, -z, -y]$	[45]
46	$[x, z, y]$	[46]
47	$[-z, y, -x]$	[47]
48	$[z, y, x]$	[48]