MSG No. 221.93 $Pm\bar{3}m1'$ [Type II, cubic]

Table 1: Wyckoff site: `1a`, site symmetry: `m-3m1'`

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,
		49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,
		73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96]

Table 2: Wyckoff site: `1b`, site symmetry: `m-3m1'`

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,
		49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,
		73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96]

Table 3: Wyckoff site: `3c`, site symmetry: `4/mm.m1'`

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,3,8,9,10,13,14,25,26,27,32,33,34,37,38,49,50,51,56,57,58,61,62,
		73,74,75,80,81,82,85,86]
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[4,5,15,16,18,19,21,23,28,29,39,40,42,43,45,47,52,53,63,64,66,67,69,71,
		76,77,87,88,90,91,93,95]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[6,7,11,12,17,20,22,24,30,31,35,36,41,44,46,48,54,55,59,60,65,68,70,72,
		78,79,83,84,89,92,94,96]

Table 4: Wyckoff site: `3d`, site symmetry: `4/mm.m1'`

No.	position	mapping
1	$\left[\frac{1}{2}, 0, 0\right]$	[1,2,3,8,9,10,13,14,25,26,27,32,33,34,37,38,49,50,51,56,57,58,61,62,
		73,74,75,80,81,82,85,86]
2	$\left[0, 0, \frac{1}{2}\right]$	[4,5,15,16,18,19,21,23,28,29,39,40,42,43,45,47,52,53,63,64,66,67,69,71,
		76,77,87,88,90,91,93,95]
3	$\left[0, \frac{1}{2}, 0\right]$	[6,7,11,12,17,20,22,24,30,31,35,36,41,44,46,48,54,55,59,60,65,68,70,72,
		78,79,83,84,89,92,94,96]

Table 5: Wyckoff site: `6e`, site symmetry: `4m.m1'`

No.	position	mapping
1	$[x, 0, 0]$	[1,2,3,8,33,34,37,38,49,50,51,56,81,82,85,86]
2	$[0, 0, -x]$	[4,16,19,23,29,39,42,45,52,64,67,71,77,87,90,93]
3	$[0, 0, x]$	[5,15,18,21,28,40,43,47,53,63,66,69,76,88,91,95]
4	$[0, x, 0]$	[6,11,17,24,31,36,44,46,54,59,65,72,79,84,92,94]
5	$[0, -x, 0]$	[7,12,20,22,30,35,41,48,55,60,68,70,78,83,89,96]
6	$[-x, 0, 0]$	[9,10,13,14,25,26,27,32,57,58,61,62,73,74,75,80]

Table 6: Wyckoff site: `6f`, site symmetry: `4m.m1'`

No.	position	mapping
1	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,3,8,33,34,37,38,49,50,51,56,81,82,85,86]
2	$\left[\frac{1}{2}, \frac{1}{2}, -x\right]$	[4,16,19,23,29,39,42,45,52,64,67,71,77,87,90,93]
3	$\left[\frac{1}{2}, \frac{1}{2}, x\right]$	[5,15,18,21,28,40,43,47,53,63,66,69,76,88,91,95]
4	$\left[\frac{1}{2}, x, \frac{1}{2}\right]$	[6,11,17,24,31,36,44,46,54,59,65,72,79,84,92,94]
5	$\left[\frac{1}{2}, -x, \frac{1}{2}\right]$	[7,12,20,22,30,35,41,48,55,60,68,70,78,83,89,96]
6	$\left[-x, \frac{1}{2}, \frac{1}{2}\right]$	[9,10,13,14,25,26,27,32,57,58,61,62,73,74,75,80]

Table 7: Wyckoff site: `8g`, site symmetry: `.3m1'`

No.	position	mapping
1	$[x, x, x]$	[1,17,18,36,38,40,49,65,66,84,86,88]
2	$[x, -x, x]$	[2,7,15,33,43,48,50,55,63,81,91,96]
3	$[x, x, -x]$	[3,4,11,34,44,45,51,52,59,82,92,93]
4	$[-x, x, x]$	[5,6,13,32,46,47,53,54,61,80,94,95]
5	$[x, -x, -x]$	[8,22,23,29,30,37,56,70,71,77,78,85]
6	$[-x, x, -x]$	[9,19,24,26,31,39,57,67,72,74,79,87]
7	$[-x, -x, x]$	[10,20,21,27,28,35,58,68,69,75,76,83]
8	$[-x, -x, -x]$	[12,14,16,25,41,42,60,62,64,73,89,90]

Table 8: Wyckoff site: `12h`, site symmetry: `2mm..1'`

No.	position	mapping
1	$\left[x, \frac{1}{2}, 0\right]$	[1,8,33,34,49,56,81,82]
2	$\left[x, 0, \frac{1}{2}\right]$	[2,3,37,38,50,51,85,86]
3	$\left[0, \frac{1}{2}, -x\right]$	[4,16,29,39,52,64,77,87]
4	$\left[0, \frac{1}{2}, x\right]$	[5,15,28,40,53,63,76,88]
5	$\left[\frac{1}{2}, x, 0\right]$	[6,11,31,36,54,59,79,84]
6	$\left[\frac{1}{2}, -x, 0\right]$	[7,12,30,35,55,60,78,83]
7	$\left[-x, \frac{1}{2}, 0\right]$	[9,10,25,32,57,58,73,80]

continued ...

Table 8

No.	position	mapping
8	$\left[-x, 0, \frac{1}{2}\right]$	[13,14,26,27,61,62,74,75]
9	$\left[0, x, \frac{1}{2}\right]$	[17,24,44,46,65,72,92,94]
10	$\left[\frac{1}{2}, 0, x\right]$	[18,21,43,47,66,69,91,95]
11	$\left[\frac{1}{2}, 0, -x\right]$	[19,23,42,45,67,71,90,93]
12	$\left[0, -x, \frac{1}{2}\right]$	[20,22,41,48,68,70,89,96]

Table 9: Wyckoff site: `12i`, site symmetry: `m.2m1'`

No.	position	mapping
1	$[0, y, y]$	[1,13,32,38,49,61,80,86]
2	$[0, -y, y]$	[2,10,27,33,50,58,75,81]
3	$[0, y, -y]$	[3,9,26,34,51,57,74,82]
4	$[y, y, 0]$	[4,18,40,45,52,66,88,93]
5	$[-y, y, 0]$	[5,19,39,47,53,67,87,95]
6	$[-y, 0, y]$	[6,20,35,46,54,68,83,94]
7	$[y, 0, y]$	[7,17,36,48,55,65,84,96]
8	$[0, -y, -y]$	[8,14,25,37,56,62,73,85]
9	$[y, 0, -y]$	[11,22,30,44,59,70,78,92]
10	$[-y, 0, -y]$	[12,24,31,41,60,72,79,89]
11	$[y, -y, 0]$	[15,23,29,43,63,71,77,91]
12	$[-y, -y, 0]$	[16,21,28,42,64,69,76,90]

Table 10: Wyckoff site: `12j`, site symmetry: `m.2m1'`

No.	position	mapping
1	$\left[\frac{1}{2}, y, y\right]$	[1,13,32,38,49,61,80,86]
2	$\left[\frac{1}{2}, -y, y\right]$	[2,10,27,33,50,58,75,81]
3	$\left[\frac{1}{2}, y, -y\right]$	[3,9,26,34,51,57,74,82]
4	$\left[y, y, \frac{1}{2}\right]$	[4,18,40,45,52,66,88,93]
5	$\left[-y, y, \frac{1}{2}\right]$	[5,19,39,47,53,67,87,95]
6	$\left[-y, \frac{1}{2}, y\right]$	[6,20,35,46,54,68,83,94]
7	$\left[y, \frac{1}{2}, y\right]$	[7,17,36,48,55,65,84,96]
8	$\left[\frac{1}{2}, -y, -y\right]$	[8,14,25,37,56,62,73,85]
9	$\left[y, \frac{1}{2}, -y\right]$	[11,22,30,44,59,70,78,92]
10	$\left[-y, \frac{1}{2}, -y\right]$	[12,24,31,41,60,72,79,89]
11	$\left[y, -y, \frac{1}{2}\right]$	[15,23,29,43,63,71,77,91]
12	$\left[-y, -y, \frac{1}{2}\right]$	[16,21,28,42,64,69,76,90]

Table 11: Wyckoff site: `24k`, site symmetry: `m..1'`

No.	position	mapping
1	$[0, y, z]$	[1,32,49,80]
2	$[0, -z, y]$	[2,27,50,75]
3	$[0, z, -y]$	[3,26,51,74]
4	$[z, y, 0]$	[4,40,52,88]
5	$[-z, y, 0]$	[5,39,53,87]
6	$[-y, 0, z]$	[6,35,54,83]
7	$[y, 0, z]$	[7,36,55,84]
8	$[0, -y, -z]$	[8,25,56,73]
9	$[0, y, -z]$	[9,34,57,82]
10	$[0, -y, z]$	[10,33,58,81]
11	$[y, 0, -z]$	[11,30,59,78]
12	$[-y, 0, -z]$	[12,31,60,79]
13	$[0, z, y]$	[13,38,61,86]
14	$[0, -z, -y]$	[14,37,62,85]
15	$[z, -y, 0]$	[15,29,63,77]
16	$[-z, -y, 0]$	[16,28,64,76]
17	$[z, 0, y]$	[17,48,65,96]
18	$[y, z, 0]$	[18,45,66,93]
19	$[-y, z, 0]$	[19,47,67,95]
20	$[-z, 0, y]$	[20,46,68,94]
21	$[-y, -z, 0]$	[21,42,69,90]
22	$[z, 0, -y]$	[22,44,70,92]
23	$[y, -z, 0]$	[23,43,71,91]
24	$[-z, 0, -y]$	[24,41,72,89]

Table 12: Wyckoff site: `24l`, site symmetry: `m..1'`

No.	position	mapping
1	$\left[\frac{1}{2}, y, z\right]$	[1,32,49,80]
2	$\left[\frac{1}{2}, -z, y\right]$	[2,27,50,75]
3	$\left[\frac{1}{2}, z, -y\right]$	[3,26,51,74]
4	$\left[z, y, \frac{1}{2}\right]$	[4,40,52,88]
5	$\left[-z, y, \frac{1}{2}\right]$	[5,39,53,87]
6	$\left[-y, \frac{1}{2}, z\right]$	[6,35,54,83]
7	$\left[y, \frac{1}{2}, z\right]$	[7,36,55,84]
8	$\left[\frac{1}{2}, -y, -z\right]$	[8,25,56,73]
9	$\left[\frac{1}{2}, y, -z\right]$	[9,34,57,82]
10	$\left[\frac{1}{2}, -y, z\right]$	[10,33,58,81]
11	$\left[y, \frac{1}{2}, -z\right]$	[11,30,59,78]
12	$\left[-y, \frac{1}{2}, -z\right]$	[12,31,60,79]
13	$\left[\frac{1}{2}, z, y\right]$	[13,38,61,86]
14	$\left[\frac{1}{2}, -z, -y\right]$	[14,37,62,85]
15	$\left[z, -y, \frac{1}{2}\right]$	[15,29,63,77]

continued …

Table 12

No.	position	mapping
16	$\left[-z, -y, \frac{1}{2}\right]$	[16,28,64,76]
17	$\left[z, \frac{1}{2}, y\right]$	[17,48,65,96]
18	$\left[y, z, \frac{1}{2}\right]$	[18,45,66,93]
19	$\left[-y, z, \frac{1}{2}\right]$	[19,47,67,95]
20	$\left[-z, \frac{1}{2}, y\right]$	[20,46,68,94]
21	$\left[-y, -z, \frac{1}{2}\right]$	[21,42,69,90]
22	$\left[z, \frac{1}{2}, -y\right]$	[22,44,70,92]
23	$\left[y, -z, \frac{1}{2}\right]$	[23,43,71,91]
24	$\left[-z, \frac{1}{2}, -y\right]$	[24,41,72,89]

Table 13: Wyckoff site: `24m`, site symmetry: `..m1`'

No.	position	mapping
1	$[x, x, z]$	[1,36,49,84]
2	$[x, -z, x]$	[2,43,50,91]
3	$[x, z, -x]$	[3,45,51,93]
4	$[z, x, -x]$	[4,44,52,92]
5	$[-z, x, x]$	[5,46,53,94]
6	$[-x, x, z]$	[6,32,54,80]
7	$[x, -x, z]$	[7,33,55,81]
8	$[x, -x, -z]$	[8,30,56,78]
9	$[-x, x, -z]$	[9,31,57,79]
10	$[-x, -x, z]$	[10,35,58,83]
11	$[x, x, -z]$	[11,34,59,82]
12	$[-x, -x, -z]$	[12,25,60,73]
13	$[-x, z, x]$	[13,47,61,95]
14	$[-x, -z, -x]$	[14,42,62,90]
15	$[z, -x, x]$	[15,48,63,96]
16	$[-z, -x, -x]$	[16,41,64,89]
17	$[z, x, x]$	[17,40,65,88]
18	$[x, z, x]$	[18,38,66,86]
19	$[-x, z, -x]$	[19,26,67,74]
20	$[-z, -x, x]$	[20,28,68,76]
21	$[-x, -z, x]$	[21,27,69,75]
22	$[z, -x, -x]$	[22,29,70,77]
23	$[x, -z, -x]$	[23,37,71,85]
24	$[-z, x, -x]$	[24,39,72,87]

Table 14: Wyckoff site: `48n`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	[1,49]
2	$[x, -z, y]$	[2,50]
3	$[x, z, -y]$	[3,51]
4	$[z, y, -x]$	[4,52]
5	$[-z, y, x]$	[5,53]
6	$[-y, x, z]$	[6,54]
7	$[y, -x, z]$	[7,55]
8	$[x, -y, -z]$	[8,56]
9	$[-x, y, -z]$	[9,57]
10	$[-x, -y, z]$	[10,58]
11	$[y, x, -z]$	[11,59]
12	$[-y, -x, -z]$	[12,60]
13	$[-x, z, y]$	[13,61]
14	$[-x, -z, -y]$	[14,62]
15	$[z, -y, x]$	[15,63]
16	$[-z, -y, -x]$	[16,64]
17	$[z, x, y]$	[17,65]
18	$[y, z, x]$	[18,66]
19	$[-y, z, -x]$	[19,67]
20	$[-z, -x, y]$	[20,68]
21	$[-y, -z, x]$	[21,69]
22	$[z, -x, -y]$	[22,70]
23	$[y, -z, -x]$	[23,71]
24	$[-z, x, -y]$	[24,72]
25	$[-x, -y, -z]$	[25,73]
26	$[-x, z, -y]$	[26,74]
27	$[-x, -z, y]$	[27,75]
28	$[-z, -y, x]$	[28,76]
29	$[z, -y, -x]$	[29,77]
30	$[y, -x, -z]$	[30,78]
31	$[-y, x, -z]$	[31,79]
32	$[-x, y, z]$	[32,80]
33	$[x, -y, z]$	[33,81]
34	$[x, y, -z]$	[34,82]
35	$[-y, -x, z]$	[35,83]
36	$[y, x, z]$	[36,84]
37	$[x, -z, -y]$	[37,85]
38	$[x, z, y]$	[38,86]
39	$[-z, y, -x]$	[39,87]
40	$[z, y, x]$	[40,88]
41	$[-z, -x, -y]$	[41,89]
42	$[-y, -z, -x]$	[42,90]
43	$[y, -z, x]$	[43,91]
44	$[z, x, -y]$	[44,92]
45	$[y, z, -x]$	[45,93]
46	$[-z, x, y]$	[46,94]

continued ...

6

Table 14

No.	position	mapping
47	$[-y,\,z,\,x]$	[47,95]
48	$[z,\,-x,\,y]$	[48,96]

| 47 | $[-y,\,z,\,x]$ | [47,95] |
| 48 | $[z,\,-x,\,y]$ | [48,96] |