MSG No. 217.79 $I\bar{4}3m1'$ [Type II, cubic]

Table 1: Wyckoff site: `2a`, site symmetry: `-43m1'`

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,
		49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72]
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,
		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: `6b`, site symmetry: `-42.m1'`

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

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

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

Table 4: Wyckoff site: `12d`, site symmetry: `-4..1'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[1,2,37,38,49,50,85,86]
2	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[3,4,45,46,51,52,93,94]
3	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[5,12,41,43,53,60,89,91]
4	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[6,9,40,47,54,57,88,95]
5	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[7,11,39,48,55,59,87,96]
6	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[8,10,42,44,56,58,90,92]
7	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[13,14,25,26,61,62,73,74]

continued ...

Table 4

No.	position	mapping
8	$\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$	[15,24,31,35,63,72,79,83]
9	$\left[0,\ \frac{1}{2},\ \frac{3}{4}\right]$	[16,23,30,33,64,71,78,81]
10	$\left[\frac{1}{2},\ \frac{3}{4},\ 0\right]$	[17,19,29,36,65,67,77,84]
11	$\left[\frac{1}{2},\ \frac{1}{4},\ 0\right]$	[18,20,32,34,66,68,80,82]
12	$\left[\frac{1}{4},\ 0,\ \frac{1}{2}\right]$	[21,22,27,28,69,70,75,76]

Table 5: Wyckoff site: 12e, site symmetry: 2.mm1'

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

Table 6: Wyckoff site: 24f, site symmetry: 2..1'

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ 0\right]$	[1,2,49,50]
2	$\left[-x,\ \frac{1}{2},\ 0\right]$	[3,4,51,52]
3	$\left[0,\ x,\ \frac{1}{2}\right]$	[5,12,53,60]
4	$\left[\frac{1}{2},\ 0,\ x\right]$	[6,9,54,57]
5	$\left[\frac{1}{2},\ 0,\ -x\right]$	[7,11,55,59]
6	$\left[0,\ -x,\ \frac{1}{2}\right]$	[8,10,56,58]
7	$\left[-x,\ 0,\ \frac{1}{2}\right]$	[13,14,61,62]
8	$\left[0,\ \frac{1}{2},\ x\right]$	[15,24,63,72]
9	$\left[0,\ \frac{1}{2},\ -x\right]$	[16,23,64,71]
10	$\left[\frac{1}{2},\ -x,\ 0\right]$	[17,19,65,67]
11	$\left[\frac{1}{2},\ x,\ 0\right]$	[18,20,66,68]
12	$\left[x,\ 0,\ \frac{1}{2}\right]$	[21,22,69,70]
13	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	[25,26,73,74]
14	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$	[27,28,75,76]
15	$\left[\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	[29,36,77,84]
16	$\left[0,\ \frac{1}{2},\ x+\frac{1}{2}\right]$	[30,33,78,81]
17	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-x\right]$	[31,35,79,83]

continued ...

Table 6

No.	position	mapping
18	$\left[\frac{1}{2},\ \frac{1}{2}-x,\ 0\right]$	[32,34,80,82]
19	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ 0\right]$	[37,38,85,86]
20	$\left[\frac{1}{2},\ 0,\ x+\frac{1}{2}\right]$	[39,48,87,96]
21	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-x\right]$	[40,47,88,95]
22	$\left[0,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[41,43,89,91]
23	$\left[0,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[42,44,90,92]
24	$\left[x+\frac{1}{2},\ \frac{1}{2},\ 0\right]$	[45,46,93,94]

Table 7: Wyckoff site: 24g, site symmetry: ..m1'

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

Table 8: Wyckoff site: 48h, site symmetry: 11'

No.	position	mapping
1	$[x,\ y,\ z]$	[1,49]
2	$[x,\ -y,\ -z]$	[2,50]
3	$[-x,\ y,\ -z]$	[3,51]

continued ...

Table 8

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