MSG No. 204.31 $Im\bar{3}1'$ [Type II, cubic]

Table 1: Wyckoff site: 2a, site symmetry: m-3.1'

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: mmm..1'

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

Table 3: Wyckoff site: 8c, site symmetry: .-3'.1'

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

Table 4: Wyckoff site: 12d, site symmetry: 2mm..1'

No.	position	mapping
1	$[x, 0, 0]$	[1,2,15,16,49,50,63,64]
2	$[-x, 0, 0]$	[3,4,13,14,51,52,61,62]
3	$[0, x, 0]$	[5,12,20,22,53,60,68,70]
4	$[0, 0, x]$	[6,9,19,23,54,57,67,71]
5	$[0, 0, -x]$	[7,11,18,21,55,59,66,69]
6	$[0, -x, 0]$	[8,10,17,24,56,58,65,72]
7	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[25,26,39,40,73,74,87,88]

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{1}{2}-x,\frac{1}{2},\frac{1}{2}\right]$	[27,28,37,38,75,76,85,86]
9	$\left[\frac{1}{2},x+\frac{1}{2},\frac{1}{2}\right]$	[29,36,44,46,77,84,92,94]
10	$\left[\frac{1}{2},\frac{1}{2},x+\frac{1}{2}\right]$	[30,33,43,47,78,81,91,95]
11	$\left[\frac{1}{2},\frac{1}{2},\frac{1}{2}-x\right]$	[31,35,42,45,79,83,90,93]
12	$\left[\frac{1}{2},\frac{1}{2}-x,\frac{1}{2}\right]$	[32,34,41,48,80,82,89,96]

Table 5: Wyckoff site: `12e`, site symmetry: `2mm..1`'

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

Table 6: Wyckoff site: `16f`, site symmetry: `.3.1`'

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

Table 7: Wyckoff site: 24g, site symmetry: m..1'

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

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]
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	$[-x, -y, -z]$	[13,61]
14	$[-x, y, z]$	[14,62]
15	$[x, -y, z]$	[15,63]

Table 8

No.	position	mapping
16	$[x, y, -z]$	[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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[25,73]
26	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[26,74]
27	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[27,75]
28	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[28,76]
29	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[29,77]
30	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[30,78]
31	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[31,79]
32	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[32,80]
33	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[33,81]
34	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[34,82]
35	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[35,83]
36	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[36,84]
37	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[37,85]
38	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[38,86]
39	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[39,87]
40	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[40,88]
41	$[\frac{1}{2} - z, \frac{1}{2} - x, \frac{1}{2} - y]$	[41,89]
42	$[\frac{1}{2} - y, \frac{1}{2} - z, \frac{1}{2} - x]$	[42,90]
43	$[y + \frac{1}{2}, \frac{1}{2} - z, x + \frac{1}{2}]$	[43,91]
44	$[z + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - y]$	[44,92]
45	$[y + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - x]$	[45,93]
46	$[\frac{1}{2} - z, x + \frac{1}{2}, y + \frac{1}{2}]$	[46,94]
47	$[\frac{1}{2} - y, z + \frac{1}{2}, x + \frac{1}{2}]$	[47,95]
48	$[z + \frac{1}{2}, \frac{1}{2} - x, y + \frac{1}{2}]$	[48,96]