MSG No. 216.76 $F\bar{4}'3m'$ [Type III, cubic]

Table 1: Wyckoff site: `4a`, site symmetry: `-4'3m'`

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]
2	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72]
4	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[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: `4b`, site symmetry: `-4'3m'`

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]
2	$\left[\frac{1}{2}, 0, 0\right]$	[25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]
3	$\left[0, \frac{1}{2}, 0\right]$	[49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72]
4	$\left[0, 0, \frac{1}{2}\right]$	[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: `4c`, site symmetry: `-4'3m'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4'3m'`

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

Table 5: Wyckoff site: `16e`, site symmetry: `.3m'`

No.	position	mapping
1	$[x, x, x]$	[1,5,6,20,22,24]
2	$[x, -x, -x]$	[2,10,11,16,17,21]

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 24g, site symmetry: 2.m'm'

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

Table 8: Wyckoff site: 48h, site symmetry: ..m'

No.	position	mapping
1	$[x,\ x,\ z]$	[1,20]
2	$[x,\ -x,\ -z]$	[2,17]
3	$[-x,\ x,\ -z]$	[3,18]
4	$[-x,\ -x,\ z]$	[4,19]
5	$[z,\ x,\ x]$	[5,24]
6	$[x,\ z,\ x]$	[6,22]
7	$[-x,\ z,\ -x]$	[7,13]
8	$[-z,\ -x,\ x]$	[8,15]
9	$[-x,\ -z,\ x]$	[9,14]
10	$[z,\ -x,\ -x]$	[10,16]
11	$[x,\ -z,\ -x]$	[11,21]
12	$[-z,\ x,\ -x]$	[12,23]
13	$\left[x,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[25,44]
14	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[26,41]
15	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[27,42]

continued ...

Table 8

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

Table 9: Wyckoff site: 96i, 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]

continued ...

Table 9

No.	position	mapping
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	$[-x, z, -y]$	[13]
14	$[-x, -z, y]$	[14]
15	$[-z, -y, x]$	[15]
16	$[z, -y, -x]$	[16]
17	$[y, -x, -z]$	[17]
18	$[-y, x, -z]$	[18]
19	$[-y, -x, z]$	[19]
20	$[y, x, z]$	[20]
21	$[x, -z, -y]$	[21]
22	$[x, z, y]$	[22]
23	$[-z, y, -x]$	[23]
24	$[z, y, x]$	[24]
25	$\left[x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[25]
26	$\left[x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[26]
27	$\left[-x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[27]
28	$\left[-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[28]
29	$\left[z, x+\frac{1}{2}, y+\frac{1}{2}\right]$	[29]
30	$\left[y, z+\frac{1}{2}, x+\frac{1}{2}\right]$	[30]
31	$\left[-y, z+\frac{1}{2}, \frac{1}{2}-x\right]$	[31]
32	$\left[-z, \frac{1}{2}-x, y+\frac{1}{2}\right]$	[32]
33	$\left[-y, \frac{1}{2}-z, x+\frac{1}{2}\right]$	[33]
34	$\left[z, \frac{1}{2}-x, \frac{1}{2}-y\right]$	[34]
35	$\left[y, \frac{1}{2}-z, \frac{1}{2}-x\right]$	[35]
36	$\left[-z, x+\frac{1}{2}, \frac{1}{2}-y\right]$	[36]
37	$\left[-x, z+\frac{1}{2}, \frac{1}{2}-y\right]$	[37]
38	$\left[-x, \frac{1}{2}-z, y+\frac{1}{2}\right]$	[38]
39	$\left[-z, \frac{1}{2}-y, x+\frac{1}{2}\right]$	[39]
40	$\left[z, \frac{1}{2}-y, \frac{1}{2}-x\right]$	[40]
41	$\left[y, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[41]
42	$\left[-y, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[42]
43	$\left[-y, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[43]
44	$\left[y, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[44]
45	$\left[x, \frac{1}{2}-z, \frac{1}{2}-y\right]$	[45]
46	$\left[x, z+\frac{1}{2}, y+\frac{1}{2}\right]$	[46]
47	$\left[-z, y+\frac{1}{2}, \frac{1}{2}-x\right]$	[47]
48	$\left[z, y+\frac{1}{2}, x+\frac{1}{2}\right]$	[48]
49	$\left[x+\frac{1}{2}, y, z+\frac{1}{2}\right]$	[49]
50	$\left[x+\frac{1}{2}, -y, \frac{1}{2}-z\right]$	[50]
51	$\left[\frac{1}{2}-x, y, \frac{1}{2}-z\right]$	[51]
52	$\left[\frac{1}{2}-x, -y, z+\frac{1}{2}\right]$	[52]
53	$\left[z+\frac{1}{2}, x, y+\frac{1}{2}\right]$	[53]
54	$\left[y+\frac{1}{2}, z, x+\frac{1}{2}\right]$	[54]

continued ...

Table 9

No.	position	mapping
55	$\left[\frac{1}{2}-y,\ z,\ \frac{1}{2}-x\right]$	[55]
56	$\left[\frac{1}{2}-z,\ -x,\ y+\frac{1}{2}\right]$	[56]
57	$\left[\frac{1}{2}-y,\ -z,\ x+\frac{1}{2}\right]$	[57]
58	$\left[z+\frac{1}{2},\ -x,\ \frac{1}{2}-y\right]$	[58]
59	$\left[y+\frac{1}{2},\ -z,\ \frac{1}{2}-x\right]$	[59]
60	$\left[\frac{1}{2}-z,\ x,\ \frac{1}{2}-y\right]$	[60]
61	$\left[\frac{1}{2}-x,\ z,\ \frac{1}{2}-y\right]$	[61]
62	$\left[\frac{1}{2}-x,\ -z,\ y+\frac{1}{2}\right]$	[62]
63	$\left[\frac{1}{2}-z,\ -y,\ x+\frac{1}{2}\right]$	[63]
64	$\left[z+\frac{1}{2},\ -y,\ \frac{1}{2}-x\right]$	[64]
65	$\left[y+\frac{1}{2},\ -x,\ \frac{1}{2}-z\right]$	[65]
66	$\left[\frac{1}{2}-y,\ x,\ \frac{1}{2}-z\right]$	[66]
67	$\left[\frac{1}{2}-y,\ -x,\ z+\frac{1}{2}\right]$	[67]
68	$\left[y+\frac{1}{2},\ x,\ z+\frac{1}{2}\right]$	[68]
69	$\left[x+\frac{1}{2},\ -z,\ \frac{1}{2}-y\right]$	[69]
70	$\left[x+\frac{1}{2},\ z,\ y+\frac{1}{2}\right]$	[70]
71	$\left[\frac{1}{2}-z,\ y,\ \frac{1}{2}-x\right]$	[71]
72	$\left[z+\frac{1}{2},\ y,\ x+\frac{1}{2}\right]$	[72]
73	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[73]
74	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[74]
75	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[75]
76	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[76]
77	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ y\right]$	[77]
78	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ x\right]$	[78]
79	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ -x\right]$	[79]
80	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ y\right]$	[80]
81	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ x\right]$	[81]
82	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ -y\right]$	[82]
83	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ -x\right]$	[83]
84	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ -y\right]$	[84]
85	$\left[\frac{1}{2}-x,\ z+\frac{1}{2},\ -y\right]$	[85]
86	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ y\right]$	[86]
87	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ x\right]$	[87]
88	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ -x\right]$	[88]
89	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ -z\right]$	[89]
90	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ -z\right]$	[90]
91	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	[91]
92	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z\right]$	[92]
93	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ -y\right]$	[93]
94	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y\right]$	[94]
95	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ -x\right]$	[95]
96	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x\right]$	[96]