MSG No. 224.113 $Pn\bar{3}m'$ [Type III, cubic]

Table 1: Wyckoff site: 2a, site symmetry: -4'3m'

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

Table 2: Wyckoff site: 4b, site symmetry: .-3m

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

Table 3: Wyckoff site: 4c, site symmetry: .-3m

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

Table 4: Wyckoff site: 6d, site symmetry: -4'2.m'

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

Table 5: Wyckoff site: 8e, site symmetry: .3m'

No.	position	mapping
1	$[x, x, x]$	[1,5,6,44,46,48]
2	$\left[x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[2,10,11,40,41,45]

continued ...

Table 5

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

Table 6: Wyckoff site: 12f, site symmetry: 2.2'2'

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

Table 7: Wyckoff site: 12g, site symmetry: 2.m'm'

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

Table 8: Wyckoff site: `24h`, site symmetry: `2..`

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

Table 9: Wyckoff site: `24i`, site symmetry: `..2'`

No.	position	mapping
1	$\left[\frac{1}{2}, y, y + \frac{1}{2}\right]$	[1,33]
2	$\left[\frac{1}{2}, \frac{1}{2} - y, -y\right]$	[2,34]
3	$[0, y, -y]$	[3,26]
4	$\left[0, \frac{1}{2} - y, y + \frac{1}{2}\right]$	[4,25]
5	$\left[y + \frac{1}{2}, \frac{1}{2}, y\right]$	[5,30]
6	$\left[y, y + \frac{1}{2}, \frac{1}{2}\right]$	[6,27]
7	$\left[\frac{1}{2} - y, y + \frac{1}{2}, 0\right]$	[7,28]
8	$[-y, 0, y]$	[8,29]
9	$\left[\frac{1}{2} - y, -y, \frac{1}{2}\right]$	[9,36]
10	$\left[y + \frac{1}{2}, 0, \frac{1}{2} - y\right]$	[10,31]
11	$[y, -y, 0]$	[11,35]
12	$\left[-y, \frac{1}{2}, \frac{1}{2} - y\right]$	[12,32]
13	$\left[\frac{1}{2}, -y, \frac{1}{2} - y\right]$	[13,45]
14	$\left[\frac{1}{2}, y + \frac{1}{2}, y\right]$	[14,46]
15	$[0, -y, y]$	[15,38]

continued ...

Table 9

No.	position	mapping
16	$\left[0,\, y+\frac{1}{2},\, \frac{1}{2}-y\right]$	[16,37]
17	$\left[\frac{1}{2}-y,\, \frac{1}{2},\, -y\right]$	[17,42]
18	$\left[-y,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[18,39]
19	$\left[y+\frac{1}{2},\, \frac{1}{2}-y,\, 0\right]$	[19,40]
20	$[y,\, 0,\, -y]$	[20,41]
21	$\left[y+\frac{1}{2},\, y,\, \frac{1}{2}\right]$	[21,48]
22	$\left[\frac{1}{2}-y,\, 0,\, y+\frac{1}{2}\right]$	[22,43]
23	$[-y,\, y,\, 0]$	[23,47]
24	$\left[y,\, \frac{1}{2},\, y+\frac{1}{2}\right]$	[24,44]

Table 10: Wyckoff site: 24j, site symmetry: ..2'

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

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

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

Table 12: Wyckoff site: `48l`, site symmetry: `1`

No.	position	mapping
1	$[x,\,y,\,z]$	[1]
2	$\left[x,\,\frac{1}{2}-y,\,\frac{1}{2}-z\right]$	[2]
3	$\left[\frac{1}{2}-x,\,y,\,\frac{1}{2}-z\right]$	[3]
4	$\left[\frac{1}{2}-x,\,\frac{1}{2}-y,\,z\right]$	[4]
5	$[z,\,x,\,y]$	[5]
6	$[y,\,z,\,x]$	[6]
7	$\left[\frac{1}{2}-y,\,z,\,\frac{1}{2}-x\right]$	[7]
8	$\left[\frac{1}{2}-z,\,\frac{1}{2}-x,\,y\right]$	[8]
9	$\left[\frac{1}{2}-y,\,\frac{1}{2}-z,\,x\right]$	[9]
10	$\left[z,\,\frac{1}{2}-x,\,\frac{1}{2}-y\right]$	[10]
11	$\left[y,\,\frac{1}{2}-z,\,\frac{1}{2}-x\right]$	[11]
12	$\left[\frac{1}{2}-z,\,x,\,\frac{1}{2}-y\right]$	[12]
13	$[-x,\,-y,\,-z]$	[13]
14	$\left[-x,\,y+\frac{1}{2},\,z+\frac{1}{2}\right]$	[14]
15	$\left[x+\frac{1}{2},\,-y,\,z+\frac{1}{2}\right]$	[15]

continued ...

Table 12

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