MSG No. 211.58 $I4'32'$ [Type III, cubic]

Table 1: Wyckoff site: 2a, site symmetry: 4'32'

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	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]

Table 2: Wyckoff site: 6b, site symmetry: 4'2.2'

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

Table 3: Wyckoff site: 8c, site symmetry: .32'

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

Table 4: Wyckoff site: 12d, site symmetry: 2.2'2'

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

continued ...

1

Table 4

No.	position	mapping
10	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[17,19,32,34]
11	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[18,20,29,36]
12	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[21,22,25,26]

Table 5: Wyckoff site: `12e`, site symmetry: `4'..`

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

Table 6: Wyckoff site: `16f`, site symmetry: `.3.`

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

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

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

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

No.	position	mapping
1	$[0, y, y]$	[1,21]
2	$[0, -y, -y]$	[2,22]
3	$[0, y, -y]$	[3,14]
4	$[0, -y, y]$	[4,13]
5	$[y, 0, y]$	[5,18]
6	$[y, y, 0]$	[6,15]
7	$[-y, y, 0]$	[7,16]
8	$[-y, 0, y]$	[8,17]
9	$[-y, -y, 0]$	[9,24]
10	$[y, 0, -y]$	[10,19]
11	$[y, -y, 0]$	[11,23]
12	$[-y, 0, -y]$	[12,20]
13	$\left[\frac{1}{2}, y+\frac{1}{2}, y+\frac{1}{2}\right]$	[25,45]
14	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-y\right]$	[26,46]
15	$\left[\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-y\right]$	[27,38]

continued ...

Table 8

No.	position	mapping
16	$\left[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}\right]$	[28,37]
17	$\left[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}\right]$	[29,42]
18	$\left[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}\right]$	[30,39]
19	$\left[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}\right]$	[31,40]
20	$\left[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}\right]$	[32,41]
21	$\left[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}\right]$	[33,48]
22	$\left[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y\right]$	[34,43]
23	$\left[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}\right]$	[35,47]
24	$\left[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y\right]$	[36,44]

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

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

Table 10: Wyckoff site: `48j`, 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]
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	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[25]
26	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[26]
27	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27]
28	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[28]
29	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[29]
30	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[30]
31	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[31]
32	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$	[32]
33	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$	[33]
34	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[34]
35	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[35]
36	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[36]
37	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, y+\frac{1}{2}\right]$	[37]
38	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, \frac{1}{2}-y\right]$	[38]
39	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[39]
40	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[40]
41	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[41]
42	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[42]
43	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[43]
44	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[44]
45	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[45]
46	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[46]

continued ...

Table 10

No.	position	mapping
47	$\left[z + \frac{1}{2},\, \frac{1}{2} - y,\, x + \frac{1}{2}\right]$	[47]
48	$\left[\frac{1}{2} - z,\, \frac{1}{2} - y,\, \frac{1}{2} - x\right]$	[48]

No.	position	mapping
47	$\left[z + \frac{1}{2},\, \frac{1}{2} - y,\, x + \frac{1}{2}\right]$	[47]
48	$\left[\frac{1}{2} - z,\, \frac{1}{2} - y,\, \frac{1}{2} - x\right]$	[48]