MSG No. 222.100 $Pn'\bar{3}'n$ [Type III, cubic]

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

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

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

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

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

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

Table 4: Wyckoff site: 12d, site symmetry: -4..

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

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[29,31,41,48]
11	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[30,32,44,46]
12	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[33,34,39,40]

Table 5: Wyckoff site: 12e, site symmetry: 4’..

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ y\right]$	`[1,33]`
2	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ \frac{1}{2}-y\right]$	`[2,34]`
3	$\left[\frac{1}{4},\ y,\ \frac{1}{2}-y\right]$	`[3,26]`
4	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ y\right]$	`[4,25]`
5	$\left[y,\ \frac{1}{4},\ y\right]$	`[5,30]`
6	$\left[y,\ y,\ \frac{1}{4}\right]$	`[6,27]`
7	$\left[\frac{1}{2}-y,\ y,\ \frac{1}{4}\right]$	`[7,28]`
8	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ y\right]$	`[8,29]`
9	$\left[\frac{1}{2}-y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	`[9,36]`
10	$\left[y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	`[10,31]`
11	$\left[y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	`[11,35]`
12	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	`[12,32]`
13	$\left[\frac{3}{4},\ y+\frac{1}{2},\ -y\right]$	`[13,40]`
14	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	`[14,39]`
15	$\left[-y,\ -y,\ \frac{3}{4}\right]$	`[15,42]`

continued ...

Table 8

No.	position	mapping
16	$\left[y+\frac{1}{2},\ -y,\ \frac{3}{4}\right]$	[16,43]
17	$\left[y+\frac{1}{2},\ \frac{3}{4},\ -y\right]$	[17,44]
18	$\left[-y,\ \frac{3}{4},\ -y\right]$	[18,41]
19	$\left[-y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[19,46]
20	$\left[y+\frac{1}{2},\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[20,48]
21	$\left[\frac{3}{4},\ -y,\ -y\right]$	[21,37]
22	$\left[\frac{3}{4},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	[22,38]
23	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[23,47]
24	$\left[y+\frac{1}{2},\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[24,45]

Table 9: Wyckoff site: 48i, 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	$\left[-x,\ z+\frac{1}{2},\ -y\right]$	[13]
14	$\left[-x,\ -z,\ y+\frac{1}{2}\right]$	[14]
15	$\left[-z,\ -y,\ x+\frac{1}{2}\right]$	[15]
16	$\left[z+\frac{1}{2},\ -y,\ -x\right]$	[16]
17	$\left[y+\frac{1}{2},\ -x,\ -z\right]$	[17]
18	$\left[-y,\ x+\frac{1}{2},\ -z\right]$	[18]
19	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[19]
20	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[20]
21	$\left[x+\frac{1}{2},\ -z,\ -y\right]$	[21]
22	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[22]
23	$\left[-z,\ y+\frac{1}{2},\ -x\right]$	[23]
24	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[24]
25	$\left[x,\ \frac{1}{2}-z,\ y\right]$	[25]
26	$\left[x,\ z,\ \frac{1}{2}-y\right]$	[26]
27	$\left[z,\ y,\ \frac{1}{2}-x\right]$	[27]
28	$\left[\frac{1}{2}-z,\ y,\ x\right]$	[28]
29	$\left[\frac{1}{2}-y,\ x,\ z\right]$	[29]
30	$\left[y,\ \frac{1}{2}-x,\ z\right]$	[30]
31	$\left[y,\ x,\ \frac{1}{2}-z\right]$	[31]

continued ...

Table 9

No.	position	mapping
32	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[32]
33	$\left[\frac{1}{2}-x,\ z,\ y\right]$	[33]
34	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[34]
35	$\left[z,\ \frac{1}{2}-y,\ x\right]$	[35]
36	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[36]
37	$[-x,\ -y,\ -z]$	[37]
38	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[38]
39	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[39]
40	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[40]
41	$[-z,\ -x,\ -y]$	[41]
42	$[-y,\ -z,\ -x]$	[42]
43	$\left[y+\frac{1}{2},\ -z,\ x+\frac{1}{2}\right]$	[43]
44	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ -y\right]$	[44]
45	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ -x\right]$	[45]
46	$\left[-z,\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$	[46]
47	$\left[-y,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[47]
48	$\left[z+\frac{1}{2},\ -x,\ y+\frac{1}{2}\right]$	[48]