MSG No. 222.101 $Pn\bar{3}n'$ [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	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[13,14,15,16,37,38,45,46]
5	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[17,20,22,24,41,42,43,44]
6	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[18,19,21,23,39,40,47,48]

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

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

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

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

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	`[18,21,28,35]`
11	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[19,23,27,36]`
12	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[20,22,30,32]`

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	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	`[15,16,45,46]`
9	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	`[17,24,41,43]`
10	$\left[\frac{3}{4}, \frac{3}{4}, -x\right]$	`[18,21,40,47]`
11	$\left[\frac{3}{4}, \frac{3}{4}, x+\frac{1}{2}\right]$	`[19,23,39,48]`
12	$\left[\frac{3}{4}, x+\frac{1}{2}, \frac{3}{4}\right]$	`[20,22,42,44]`

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	$[-x, -x, -x]$	`[13,17,18]`
6	$\left[-x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	`[14,22,23]`
7	$\left[x+\frac{1}{2}, -x, x+\frac{1}{2}\right]$	`[15,19,24]`
8	$\left[x+\frac{1}{2}, x+\frac{1}{2}, -x\right]$	`[16,20,21]`
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	$\left[-x, x+\frac{1}{2}, -x\right]$	`[37,42,47]`
14	$\left[-x, -x, x+\frac{1}{2}\right]$	`[38,39,43]`
15	$\left[x+\frac{1}{2}, -x, -x\right]$	`[40,41,45]`
16	$\left[x+\frac{1}{2}, x+\frac{1}{2}, x+\frac{1}{2}\right]$	`[44,46,48]`

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	$\left[-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	[13,14]
8	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{3}{4}\right]$	[15,16]
9	$\left[\frac{3}{4},\ -x,\ \frac{1}{4}\right]$	[17,24]
10	$\left[\frac{1}{4},\ \frac{3}{4},\ -x\right]$	[18,21]
11	$\left[\frac{1}{4},\ \frac{3}{4},\ x+\frac{1}{2}\right]$	[19,23]
12	$\left[\frac{3}{4},\ x+\frac{1}{2},\ \frac{1}{4}\right]$	[20,22]
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	$\left[-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[37,38]
20	$\left[\frac{3}{4},\ \frac{1}{4},\ x+\frac{1}{2}\right]$	[39,48]
21	$\left[\frac{3}{4},\ \frac{1}{4},\ -x\right]$	[40,47]
22	$\left[\frac{1}{4},\ -x,\ \frac{3}{4}\right]$	[41,43]
23	$\left[\frac{1}{4},\ x+\frac{1}{2},\ \frac{3}{4}\right]$	[42,44]
24	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$	[45,46]

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	$\left[\frac{3}{4},\ -y,\ -y\right]$	[13,45]
14	$\left[\frac{3}{4},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	[14,46]
15	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	[15,38]

continued ...

Table 8

No.	position	mapping
16	$\left[\frac{3}{4}, y+\frac{1}{2}, -y\right]$	[16,37]
17	$\left[-y, \frac{3}{4}, -y\right]$	[17,42]
18	$\left[-y, -y, \frac{3}{4}\right]$	[18,39]
19	$\left[y+\frac{1}{2}, -y, \frac{3}{4}\right]$	[19,40]
20	$\left[y+\frac{1}{2}, \frac{3}{4}, -y\right]$	[20,41]
21	$\left[y+\frac{1}{2}, y+\frac{1}{2}, \frac{3}{4}\right]$	[21,48]
22	$\left[-y, \frac{3}{4}, y+\frac{1}{2}\right]$	[22,43]
23	$\left[-y, y+\frac{1}{2}, \frac{3}{4}\right]$	[23,47]
24	$\left[y+\frac{1}{2}, \frac{3}{4}, y+\frac{1}{2}\right]$	[24,44]

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	$[-x, -y, -z]$	[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]
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	$\left[x, \frac{1}{2}-z, y\right]$	[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	$\left[-x,\ z+\frac{1}{2},\ -y\right]$	[37]
38	$\left[-x,\ -z,\ y+\frac{1}{2}\right]$	[38]
39	$\left[-z,\ -y,\ x+\frac{1}{2}\right]$	[39]
40	$\left[z+\frac{1}{2},\ -y,\ -x\right]$	[40]
41	$\left[y+\frac{1}{2},\ -x,\ -z\right]$	[41]
42	$\left[-y,\ x+\frac{1}{2},\ -z\right]$	[42]
43	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[43]
44	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[44]
45	$\left[x+\frac{1}{2},\ -z,\ -y\right]$	[45]
46	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[46]
47	$\left[-z,\ y+\frac{1}{2},\ -x\right]$	[47]
48	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[48]