MSG No. 222.98 $Pn\bar{3}n$ [Type I, cubic]

Table 1: Wyckoff site: 2a, site symmetry: 432

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24]
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[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: 42.2

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

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

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

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

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

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[18,21,29,39]
11	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[19,23,28,40]
12	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[20,22,31,36]

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

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

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

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

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

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

continued ...

Table 8

No.	position	mapping
16	$\left[-y,\ -y,\ \frac{3}{4}\right]$	[28,42]
17	$\left[y+\frac{1}{2},\ -y,\ \frac{3}{4}\right]$	[29,43]
18	$\left[y+\frac{1}{2},\ \frac{3}{4},\ -y\right]$	[30,44]
19	$\left[-y,\ \frac{3}{4},\ -y\right]$	[31,41]
20	$\left[\frac{3}{4},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	[32,38]
21	$\left[-y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[35,46]
22	$\left[y+\frac{1}{2},\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[36,48]
23	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[39,47]
24	$\left[y+\frac{1}{2},\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[40,45]

Table 9: Wyckoff site: 48i, site symmetry: 1

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