MSG No. 201.21 $P_In\bar{3}$ [Type IV, cubic]

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

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[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	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[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: 6b, site symmetry: m'm'm'..

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

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	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[25,29,30,37,41,42]
6	$\left[\frac{1}{2}, 0, 0\right]$	[26,34,35,38,46,47]
7	$\left[0, \frac{1}{2}, 0\right]$	[27,31,36,39,43,48]
8	$\left[0, 0, \frac{1}{2}\right]$	[28,32,33,40,44,45]

Table 4: Wyckoff site: 12d, site symmetry: 2m'm'..

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

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{4}, \frac{1}{4}, -x\right]$	[18,21,31,35]
11	$\left[\frac{1}{4}, \frac{1}{4}, x+\frac{1}{2}\right]$	[19,23,30,33]
12	$\left[\frac{1}{4}, x+\frac{1}{2}, \frac{1}{4}\right]$	[20,22,29,36]

Table 5: Wyckoff site: 12e, site symmetry: 2m'm'..

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

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	$\left[x+\frac{1}{2}, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[25,29,30]
10	$\left[x+\frac{1}{2}, -x, -x\right]$	[26,34,35]
11	$\left[-x, x+\frac{1}{2}, -x\right]$	[27,31,36]
12	$\left[-x, -x, x+\frac{1}{2}\right]$	[28,32,33]
13	$\left[\frac{1}{2}-x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[37,41,42]
14	$\left[\frac{1}{2}-x, x, x\right]$	[38,46,47]
15	$\left[x, \frac{1}{2}-x, x\right]$	[39,43,48]
16	$\left[x, x, \frac{1}{2}-x\right]$	[40,44,45]

Table 7: Wyckoff site: 24g, site symmetry: m’..

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

Table 8: Wyckoff site: 48h, 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 8

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