MSG No. 218.84 $P_I\bar{4}3n$ [Type IV, cubic]

Table 1: Wyckoff site: `2a`, site symmetry: `-4'3m'`

No.	position	mapping
1	$[0, 0, 0]$	[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	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[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: `-4'2.m'`

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

Table 3: Wyckoff site: `8c`, site symmetry: `.3m'`

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

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

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

Table 4

No.	position	mapping
10	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[30,33,40,47]
11	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[31,35,39,48]
12	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[32,34,42,44]

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

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

Table 6: Wyckoff site: 24f, 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	$\left[\frac{1}{2} - x, \frac{1}{2}, 0\right]$	[13,14]
8	$\left[\frac{1}{2}, 0, x + \frac{1}{2}\right]$	[15,24]
9	$\left[\frac{1}{2}, 0, \frac{1}{2} - x\right]$	[16,23]
10	$\left[0, \frac{1}{2} - x, \frac{1}{2}\right]$	[17,19]
11	$\left[0, x + \frac{1}{2}, \frac{1}{2}\right]$	[18,20]
12	$\left[x + \frac{1}{2}, \frac{1}{2}, 0\right]$	[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	$\left[-x, 0, \frac{1}{2}\right]$	[37,38]

continued ...

Table 6

No.	position	mapping
20	$\left[0, \frac{1}{2}, x\right]$	[39,48]
21	$\left[0, \frac{1}{2}, -x\right]$	[40,47]
22	$\left[\frac{1}{2}, -x, 0\right]$	[41,43]
23	$\left[\frac{1}{2}, x, 0\right]$	[42,44]
24	$\left[x, 0, \frac{1}{2}\right]$	[45,46]

Table 7: Wyckoff site: `24g`, site symmetry: `..m'`

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

Table 8: Wyckoff site: `48h`, 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]

continued ...

Table 8

No.	position	mapping
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	$\left[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y\right]$	[13]
14	$\left[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}\right]$	[14]
15	$\left[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}\right]$	[15]
16	$\left[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x\right]$	[16]
17	$\left[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z\right]$	[17]
18	$\left[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z\right]$	[18]
19	$\left[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}\right]$	[19]
20	$\left[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}\right]$	[20]
21	$\left[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y\right]$	[21]
22	$\left[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}\right]$	[22]
23	$\left[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x\right]$	[23]
24	$\left[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}\right]$	[24]
25	$\left[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[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	$[-x, z, -y]$	[37]
38	$[-x, -z, y]$	[38]
39	$[-z, -y, x]$	[39]
40	$[z, -y, -x]$	[40]
41	$[y, -x, -z]$	[41]
42	$[-y, x, -z]$	[42]
43	$[-y, -x, z]$	[43]
44	$[y, x, z]$	[44]
45	$[x, -z, -y]$	[45]
46	$[x, z, y]$	[46]
47	$[-z, y, -x]$	[47]
48	$[z, y, x]$	[48]