MSG No. 215.73 $P_I\bar{4}3m$ [Type IV, cubic]

Table 1: Wyckoff site: `2a`, site symmetry: `-43m`

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{2},\ 0\right]$	`[1,2,37,38]`
2	$\left[\frac{3}{4},\ \frac{1}{2},\ 0\right]$	`[3,4,45,46]`
3	$\left[0,\ \frac{1}{4},\ \frac{1}{2}\right]$	`[5,12,41,43]`
4	$\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$	`[6,9,40,47]`
5	$\left[\frac{1}{2},\ 0,\ \frac{3}{4}\right]$	`[7,11,39,48]`
6	$\left[0,\ \frac{3}{4},\ \frac{1}{2}\right]$	`[8,10,42,44]`
7	$\left[\frac{3}{4},\ 0,\ \frac{1}{2}\right]$	`[13,14,25,26]`
8	$\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[15,24,31,35]`
9	$\left[0,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[16,23,30,33]`

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	`[17,19,29,36]`
11	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	`[18,20,32,34]`
12	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	`[21,22,27,28]`

Table 5: Wyckoff site: `12e`, site symmetry: `2.mm`

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

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

continued ...

Table 6

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

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

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

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