MSG No. 224.110 $Pn\bar{3}m$ [Type I, cubic]

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

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

Table 2: Wyckoff site: 4b, site symmetry: .-3m

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

Table 3: Wyckoff site: 4c, site symmetry: .-3m

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

Table 4: Wyckoff site: 6d, site symmetry: -42.m

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

Table 5: Wyckoff site: 8e, site symmetry: .3m

No.	position	mapping
1	$[x, x, x]$	[1,17,18,36,38,40]
2	$\left[x+\frac{1}{2}, -x, x+\frac{1}{2}\right]$	[2,7,15,33,43,48]

continued ...

Table 5

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

Table 6: Wyckoff site: 12f, site symmetry: 2.22

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

Table 7: Wyckoff site: 12g, site symmetry: 2.mm

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

Table 8: Wyckoff site: `24h`, site symmetry: `2..`

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

Table 9: Wyckoff site: `24i`, site symmetry: `..2`

No.	position	mapping
1	$\left[\frac{1}{2},\ y,\ y+\frac{1}{2}\right]$	`[1,13]`
2	$\left[0,\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	`[2,10]`
3	$[0,\ y,\ -y]$	`[3,9]`
4	$\left[y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[4,18]`
5	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ 0\right]$	`[5,19]`
6	$[-y,\ 0,\ y]$	`[6,20]`
7	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y\right]$	`[7,17]`
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -y\right]$	`[8,14]`
9	$\left[y+\frac{1}{2},\ 0,\ \frac{1}{2}-y\right]$	`[11,22]`
10	$\left[-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	`[12,24]`
11	$[y,\ -y,\ 0]$	`[15,23]`
12	$\left[\frac{1}{2}-y,\ -y,\ \frac{1}{2}\right]$	`[16,21]`
13	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}-y\right]$	`[25,37]`
14	$\left[0,\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	`[26,34]`
15	$[0,\ -y,\ y]$	`[27,33]`

continued ...

Table 9

No.	position	mapping
16	$\left[-y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[28,42]
17	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[29,43]
18	$[y,\ 0,\ -y]$	[30,44]
19	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ -y\right]$	[31,41]
20	$\left[\frac{1}{2},\ y+\frac{1}{2},\ y\right]$	[32,38]
21	$\left[\frac{1}{2}-y,\ 0,\ y+\frac{1}{2}\right]$	[35,46]
22	$\left[y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[36,48]
23	$[-y,\ y,\ 0]$	[39,47]
24	$\left[y+\frac{1}{2},\ y,\ \frac{1}{2}\right]$	[40,45]

Table 10: Wyckoff site: 24j, site symmetry: ..2

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

Table 11: Wyckoff site: `24k`, site symmetry: `..m`

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

Table 12: Wyckoff site: `48l`, site symmetry: `1`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1]`
2	$\left[x+\frac{1}{2},\ -z,\ y+\frac{1}{2}\right]$	`[2]`
3	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ -y\right]$	`[3]`
4	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ -x\right]$	`[4]`
5	$\left[-z,\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	`[5]`
6	$\left[-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[6]`
7	$\left[y+\frac{1}{2},\ -x,\ z+\frac{1}{2}\right]$	`[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	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	`[11]`
12	$[-y,\ -x,\ -z]$	`[12]`
13	$\left[-x,\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	`[13]`
14	$[-x,\ -z,\ -y]$	`[14]`
15	$\left[z+\frac{1}{2},\ -y,\ x+\frac{1}{2}\right]$	`[15]`

continued ...

Table 12

No.	position	mapping
16	$[-z,\ -y,\ -x]$	[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	$\left[\frac{1}{2}-x,\ z,\ \frac{1}{2}-y\right]$	[26]
27	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ y\right]$	[27]
28	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ x\right]$	[28]
29	$\left[z,\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[29]
30	$\left[y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\ x,\ \frac{1}{2}-z\right]$	[31]
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	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	[35]
36	$[y,\ x,\ z]$	[36]
37	$\left[x,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[37]
38	$[x,\ z,\ y]$	[38]
39	$\left[\frac{1}{2}-z,\ y,\ \frac{1}{2}-x\right]$	[39]
40	$[z,\ y,\ x]$	[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]