MSG No. 220.91 $I\bar{4}'3d'$ [Type III, cubic]

Table 1: Wyckoff site: `12a`, site symmetry: `-4'..`

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

Table 2: Wyckoff site: `12b`, site symmetry: `-4'..`

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

Table 3: Wyckoff site: `16c`, site symmetry: `.3.`

No.	position	mapping
1	$[x, x, x]$	`[1,5,6]`
2	$\left[x, -x, \frac{1}{2} - x\right]$	`[2,10,11]`
3	$\left[\frac{1}{2} - x, x, -x\right]$	`[3,7,12]`
4	$\left[-x, \frac{1}{2} - x, x\right]$	`[4,8,9]`
5	$\left[\frac{1}{4} - x, x + \frac{1}{4}, \frac{3}{4} - x\right]$	`[13,18,23]`
6	$\left[\frac{3}{4} - x, \frac{1}{4} - x, x + \frac{1}{4}\right]$	`[14,15,19]`
7	$\left[x + \frac{1}{4}, \frac{3}{4} - x, \frac{1}{4} - x\right]$	`[16,17,21]`

continued ...

Table 3

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

Table 4: Wyckoff site: 24d, site symmetry: 2..

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

Table 5: Wyckoff site: 48e, site symmetry: 1

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

continued ...

Table 5

No.	position	mapping
47	$\left[\frac{3}{4}-z,\, y+\frac{3}{4},\, \frac{1}{4}-x\right]$	[47]
48	$\left[z+\frac{3}{4},\, y+\frac{3}{4},\, x+\frac{3}{4}\right]$	[48]