MSG No. 220.90 $\,I\bar{4}3d1'$ [Type II, cubic]

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

No.	position	mapping
1	$\left[\frac{3}{8}, 0, \frac{1}{4}\right]$	[1,2,14,37,49,50,62,85]
2	$\left[\frac{1}{8}, 0, \frac{3}{4}\right]$	[3,28,45,46,51,76,93,94]
3	$\left[\frac{5}{8}, \frac{1}{2}, \frac{1}{4}\right]$	[4,21,22,27,52,69,70,75]
4	$\left[\frac{1}{4}, \frac{3}{8}, 0\right]$	[5,12,17,43,53,60,65,91]
5	$\left[0, \frac{1}{4}, \frac{3}{8}\right]$	[6,9,23,40,54,57,71,88]
6	$\left[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}\right]$	[7,15,24,35,55,63,72,83]
7	$\left[\frac{3}{4}, \frac{1}{8}, 0\right]$	[8,34,42,44,56,82,90,92]
8	$\left[\frac{1}{4}, \frac{5}{8}, \frac{1}{2}\right]$	[10,18,20,32,58,66,68,80]
9	$\left[0, \frac{3}{4}, \frac{1}{8}\right]$	[11,31,39,48,59,79,87,96]
10	$\left[\frac{7}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[13,25,26,38,61,73,74,86]
11	$\left[\frac{1}{2}, \frac{3}{4}, \frac{7}{8}\right]$	[16,30,33,47,64,78,81,95]
12	$\left[\frac{3}{4}, \frac{7}{8}, \frac{1}{2}\right]$	[19,29,36,41,67,77,84,89]

Table 2: Wyckoff site: `12b`, site symmetry: `-4..1'`

No.	position	mapping
1	$\left[\frac{7}{8}, 0, \frac{1}{4}\right]$	[1,2,14,37,49,50,62,85]
2	$\left[\frac{5}{8}, 0, \frac{3}{4}\right]$	[3,28,45,46,51,76,93,94]
3	$\left[\frac{1}{8}, \frac{1}{2}, \frac{1}{4}\right]$	[4,21,22,27,52,69,70,75]
4	$\left[\frac{1}{4}, \frac{7}{8}, 0\right]$	[5,12,17,43,53,60,65,91]
5	$\left[0, \frac{1}{4}, \frac{7}{8}\right]$	[6,9,23,40,54,57,71,88]
6	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{8}\right]$	[7,15,24,35,55,63,72,83]
7	$\left[\frac{3}{4}, \frac{5}{8}, 0\right]$	[8,34,42,44,56,82,90,92]
8	$\left[\frac{1}{4}, \frac{1}{8}, \frac{1}{2}\right]$	[10,18,20,32,58,66,68,80]
9	$\left[0, \frac{3}{4}, \frac{5}{8}\right]$	[11,31,39,48,59,79,87,96]
10	$\left[\frac{3}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[13,25,26,38,61,73,74,86]
11	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}\right]$	[16,30,33,47,64,78,81,95]
12	$\left[\frac{3}{4}, \frac{3}{8}, \frac{1}{2}\right]$	[19,29,36,41,67,77,84,89]

Table 3: Wyckoff site: `16c`, site symmetry: `.3.1'`

No.	position	mapping
1	$[x, x, x]$	[1,5,6,49,53,54]
2	$\left[x, -x, \frac{1}{2} - x\right]$	[2,10,11,50,58,59]
3	$\left[\frac{1}{2} - x, x, -x\right]$	[3,7,12,51,55,60]
4	$\left[-x, \frac{1}{2} - x, x\right]$	[4,8,9,52,56,57]
5	$\left[\frac{1}{4} - x, x + \frac{1}{4}, \frac{3}{4} - x\right]$	[13,18,23,61,66,71]
6	$\left[\frac{3}{4} - x, \frac{1}{4} - x, x + \frac{1}{4}\right]$	[14,15,19,62,63,67]
7	$\left[x + \frac{1}{4}, \frac{3}{4} - x, \frac{1}{4} - x\right]$	[16,17,21,64,65,69]

continued ...

Table 3

No.	position	mapping
8	$\left[x+\frac{1}{4},\, x+\frac{1}{4},\, x+\frac{1}{4}\right]$	[20,22,24,68,70,72]
9	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, x+\frac{1}{2}\right]$	[25,29,30,73,77,78]
10	$\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, -x\right]$	[26,34,35,74,82,83]
11	$\left[-x,\, x+\frac{1}{2},\, \frac{1}{2}-x\right]$	[27,31,36,75,79,84]
12	$\left[\frac{1}{2}-x,\, -x,\, x+\frac{1}{2}\right]$	[28,32,33,76,80,81]
13	$\left[\frac{3}{4}-x,\, x+\frac{3}{4},\, \frac{1}{4}-x\right]$	[37,42,47,85,90,95]
14	$\left[\frac{1}{4}-x,\, \frac{3}{4}-x,\, x+\frac{3}{4}\right]$	[38,39,43,86,87,91]
15	$\left[x+\frac{3}{4},\, \frac{1}{4}-x,\, \frac{3}{4}-x\right]$	[40,41,45,88,89,93]
16	$\left[x+\frac{3}{4},\, x+\frac{3}{4},\, x+\frac{3}{4}\right]$	[44,46,48,92,94,96]

Table 4: Wyckoff site: 24d, site symmetry: 2..1'

No.	position	mapping
1	$\left[x,\, 0,\, \frac{1}{4}\right]$	[1,2,49,50]
2	$\left[\frac{1}{2}-x,\, 0,\, \frac{3}{4}\right]$	[3,28,51,76]
3	$\left[-x,\, \frac{1}{2},\, \frac{1}{4}\right]$	[4,27,52,75]
4	$\left[\frac{1}{4},\, x,\, 0\right]$	[5,12,53,60]
5	$\left[0,\, \frac{1}{4},\, x\right]$	[6,9,54,57]
6	$\left[\frac{1}{2},\, \frac{1}{4},\, -x\right]$	[7,35,55,83]
7	$\left[\frac{3}{4},\, \frac{1}{2}-x,\, 0\right]$	[8,34,56,82]
8	$\left[\frac{1}{4},\, -x,\, \frac{1}{2}\right]$	[10,32,58,80]
9	$\left[0,\, \frac{3}{4},\, \frac{1}{2}-x\right]$	[11,31,59,79]
10	$\left[\frac{1}{4}-x,\, \frac{1}{2},\, \frac{3}{4}\right]$	[13,38,61,86]
11	$\left[\frac{3}{4}-x,\, 0,\, \frac{1}{4}\right]$	[14,37,62,85]
12	$\left[\frac{1}{2},\, \frac{1}{4},\, x+\frac{1}{4}\right]$	[15,24,63,72]
13	$\left[\frac{1}{2},\, \frac{3}{4},\, \frac{1}{4}-x\right]$	[16,47,64,95]
14	$\left[\frac{1}{4},\, \frac{3}{4}-x,\, 0\right]$	[17,43,65,91]
15	$\left[\frac{1}{4},\, x+\frac{1}{4},\, \frac{1}{2}\right]$	[18,20,66,68]
16	$\left[\frac{3}{4},\, \frac{1}{4}-x,\, \frac{1}{2}\right]$	[19,41,67,89]
17	$\left[x+\frac{1}{4},\, \frac{1}{2},\, \frac{1}{4}\right]$	[21,22,69,70]
18	$\left[0,\, \frac{1}{4},\, \frac{3}{4}-x\right]$	[23,40,71,88]
19	$\left[x+\frac{1}{2},\, \frac{1}{2},\, \frac{3}{4}\right]$	[25,26,73,74]
20	$\left[\frac{3}{4},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	[29,36,77,84]
21	$\left[\frac{1}{2},\, \frac{3}{4},\, x+\frac{1}{2}\right]$	[30,33,78,81]
22	$\left[0,\, \frac{3}{4},\, x+\frac{3}{4}\right]$	[39,48,87,96]
23	$\left[\frac{3}{4},\, x+\frac{3}{4},\, 0\right]$	[42,44,90,92]
24	$\left[x+\frac{3}{4},\, 0,\, \frac{3}{4}\right]$	[45,46,93,94]

Table 5: Wyckoff site: `48e`, site symmetry: `11'`

No.	position	mapping
1	$[x,\, y,\, z]$	[1,49]
2	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	[2,50]
3	$\left[\frac{1}{2}-x,\, y,\, -z\right]$	[3,51]
4	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	[4,52]
5	$[z,\, x,\, y]$	[5,53]
6	$[y,\, z,\, x]$	[6,54]
7	$\left[\frac{1}{2}-y,\, z,\, -x\right]$	[7,55]
8	$\left[-z,\, \frac{1}{2}-x,\, y\right]$	[8,56]
9	$\left[-y,\, \frac{1}{2}-z,\, x\right]$	[9,57]
10	$\left[z,\, -x,\, \frac{1}{2}-y\right]$	[10,58]
11	$\left[y,\, -z,\, \frac{1}{2}-x\right]$	[11,59]
12	$\left[\frac{1}{2}-z,\, x,\, -y\right]$	[12,60]
13	$\left[\frac{1}{4}-x,\, z+\frac{1}{4},\, \frac{3}{4}-y\right]$	[13,61]
14	$\left[\frac{3}{4}-x,\, \frac{1}{4}-z,\, y+\frac{1}{4}\right]$	[14,62]
15	$\left[\frac{3}{4}-z,\, \frac{1}{4}-y,\, x+\frac{1}{4}\right]$	[15,63]
16	$\left[z+\frac{1}{4},\, \frac{3}{4}-y,\, \frac{1}{4}-x\right]$	[16,64]
17	$\left[y+\frac{1}{4},\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[17,65]
18	$\left[\frac{1}{4}-y,\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[18,66]
19	$\left[\frac{3}{4}-y,\, \frac{1}{4}-x,\, z+\frac{1}{4}\right]$	[19,67]
20	$\left[y+\frac{1}{4},\, x+\frac{1}{4},\, z+\frac{1}{4}\right]$	[20,68]
21	$\left[x+\frac{1}{4},\, \frac{3}{4}-z,\, \frac{1}{4}-y\right]$	[21,69]
22	$\left[x+\frac{1}{4},\, z+\frac{1}{4},\, y+\frac{1}{4}\right]$	[22,70]
23	$\left[\frac{1}{4}-z,\, y+\frac{1}{4},\, \frac{3}{4}-x\right]$	[23,71]
24	$\left[z+\frac{1}{4},\, y+\frac{1}{4},\, x+\frac{1}{4}\right]$	[24,72]
25	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[25,73]
26	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[26,74]
27	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27,75]
28	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[28,76]
29	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[29,77]
30	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[30,78]
31	$\left[-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[31,79]
32	$\left[\frac{1}{2}-z,\, -x,\, y+\frac{1}{2}\right]$	[32,80]
33	$\left[\frac{1}{2}-y,\, -z,\, x+\frac{1}{2}\right]$	[33,81]
34	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -y\right]$	[34,82]
35	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, -x\right]$	[35,83]
36	$\left[-z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[36,84]
37	$\left[\frac{3}{4}-x,\, z+\frac{3}{4},\, \frac{1}{4}-y\right]$	[37,85]
38	$\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, y+\frac{3}{4}\right]$	[38,86]
39	$\left[\frac{1}{4}-z,\, \frac{3}{4}-y,\, x+\frac{3}{4}\right]$	[39,87]
40	$\left[z+\frac{3}{4},\, \frac{1}{4}-y,\, \frac{3}{4}-x\right]$	[40,88]
41	$\left[y+\frac{3}{4},\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[41,89]
42	$\left[\frac{3}{4}-y,\, x+\frac{3}{4},\, \frac{1}{4}-z\right]$	[42,90]
43	$\left[\frac{1}{4}-y,\, \frac{3}{4}-x,\, z+\frac{3}{4}\right]$	[43,91]
44	$\left[y+\frac{3}{4},\, x+\frac{3}{4},\, z+\frac{3}{4}\right]$	[44,92]
45	$\left[x+\frac{3}{4},\, \frac{1}{4}-z,\, \frac{3}{4}-y\right]$	[45,93]
46	$\left[x+\frac{3}{4},\, z+\frac{3}{4},\, y+\frac{3}{4}\right]$	[46,94]

Table 5

No.	position	mapping
47	$\left[\frac{3}{4} - z,\, y + \frac{3}{4},\, \frac{1}{4} - x\right]$	[47,95]
48	$\left[z + \frac{3}{4},\, y + \frac{3}{4},\, x + \frac{3}{4}\right]$	[48,96]

47	$\left[\frac{3}{4} - z,\, y + \frac{3}{4},\, \frac{1}{4} - x\right]$	[47,95]
48	$\left[z + \frac{3}{4},\, y + \frac{3}{4},\, x + \frac{3}{4}\right]$	[48,96]