MSG No. 206.38 $Ia\bar{3}1'$ [Type II, cubic]

Table 1: Wyckoff site: 8a, site symmetry: .-3'.1'

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

Table 2: Wyckoff site: 8b, site symmetry: .-3'.1'

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

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	$[-x,\ -x,\ -x]$	[13,17,18,61,65,66]
6	$\left[-x,\ x,\ x+\frac{1}{2}\right]$	[14,22,23,62,70,71]
7	$\left[x+\frac{1}{2},\ -x,\ x\right]$	[15,19,24,63,67,72]
8	$\left[x,\ x+\frac{1}{2},\ -x\right]$	[16,20,21,64,68,69]
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	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[37,41,42,85,89,90]
14	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ x\right]$	[38,46,47,86,94,95]
15	$\left[x,\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	[39,43,48,87,91,96]

continued ...

Table 3

No.	position	mapping
16	$\left[x+\frac{1}{2},\, x,\, \frac{1}{2}-x\right]$	[40,44,45,88,92,93]

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	$\left[-x,\, 0,\, \frac{3}{4}\right]$	[13,14,61,62]
11	$\left[x+\frac{1}{2},\, 0,\, \frac{1}{4}\right]$	[15,40,63,88]
12	$\left[x,\, \frac{1}{2},\, \frac{3}{4}\right]$	[16,39,64,87]
13	$\left[\frac{3}{4},\, -x,\, 0\right]$	[17,24,65,72]
14	$\left[0,\, \frac{3}{4},\, -x\right]$	[18,21,66,69]
15	$\left[\frac{1}{2},\, \frac{3}{4},\, x\right]$	[19,47,67,95]
16	$\left[\frac{1}{4},\, x+\frac{1}{2},\, 0\right]$	[20,46,68,94]
17	$\left[\frac{3}{4},\, x,\, \frac{1}{2}\right]$	[22,44,70,92]
18	$\left[0,\, \frac{1}{4},\, x+\frac{1}{2}\right]$	[23,43,71,91]
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	$\left[\frac{1}{2}-x,\, \frac{1}{2},\, \frac{1}{4}\right]$	[37,38,85,86]
23	$\left[\frac{1}{4},\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[41,48,89,96]
24	$\left[\frac{1}{2},\, \frac{1}{4},\, \frac{1}{2}-x\right]$	[42,45,90,93]

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]

continued ...

Table 5

No.	position	mapping
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	$[-x,\,-y,\,-z]$	[13,61]
14	$\left[-x,\,y,\,z+\frac{1}{2}\right]$	[14,62]
15	$\left[x+\frac{1}{2},\,-y,\,z\right]$	[15,63]
16	$\left[x,\,y+\frac{1}{2},\,-z\right]$	[16,64]
17	$[-z,\,-x,\,-y]$	[17,65]
18	$[-y,\,-z,\,-x]$	[18,66]
19	$\left[y+\frac{1}{2},\,-z,\,x\right]$	[19,67]
20	$\left[z,\,x+\frac{1}{2},\,-y\right]$	[20,68]
21	$\left[y,\,z+\frac{1}{2},\,-x\right]$	[21,69]
22	$\left[-z,\,x,\,y+\frac{1}{2}\right]$	[22,70]
23	$\left[-y,\,z,\,x+\frac{1}{2}\right]$	[23,71]
24	$\left[z+\frac{1}{2},\,-x,\,y\right]$	[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	$\left[\frac{1}{2}-x,\,\frac{1}{2}-y,\,\frac{1}{2}-z\right]$	[37,85]
38	$\left[\frac{1}{2}-x,\,y+\frac{1}{2},\,z\right]$	[38,86]
39	$\left[x,\,\frac{1}{2}-y,\,z+\frac{1}{2}\right]$	[39,87]
40	$\left[x+\frac{1}{2},\,y,\,\frac{1}{2}-z\right]$	[40,88]
41	$\left[\frac{1}{2}-z,\,\frac{1}{2}-x,\,\frac{1}{2}-y\right]$	[41,89]
42	$\left[\frac{1}{2}-y,\,\frac{1}{2}-z,\,\frac{1}{2}-x\right]$	[42,90]
43	$\left[y,\,\frac{1}{2}-z,\,x+\frac{1}{2}\right]$	[43,91]
44	$\left[z+\frac{1}{2},\,x,\,\frac{1}{2}-y\right]$	[44,92]
45	$\left[y+\frac{1}{2},\,z,\,\frac{1}{2}-x\right]$	[45,93]
46	$\left[\frac{1}{2}-z,\,x+\frac{1}{2},\,y\right]$	[46,94]
47	$\left[\frac{1}{2}-y,\,z+\frac{1}{2},\,x\right]$	[47,95]
48	$\left[z,\,\frac{1}{2}-x,\,y+\frac{1}{2}\right]$	[48,96]