MSG No. 206.37 $Ia\bar{3}$ [Type I, cubic]

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

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

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

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

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	$[-x, -x, -x]$	[13,17,18]
6	$\left[-x, x, x + \frac{1}{2}\right]$	[14,22,23]
7	$\left[x + \frac{1}{2}, -x, x\right]$	[15,19,24]
8	$\left[x, x + \frac{1}{2}, -x\right]$	[16,20,21]
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	$\left[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[37,41,42]
14	$\left[\frac{1}{2} - x, x + \frac{1}{2}, x\right]$	[38,46,47]
15	$\left[x, \frac{1}{2} - x, x + \frac{1}{2}\right]$	[39,43,48]

Table 3

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

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	$\left[-x,\, 0,\, \frac{3}{4}\right]$	[13,14]
11	$\left[x + \frac{1}{2},\, 0,\, \frac{1}{4}\right]$	[15,40]
12	$\left[x,\, \frac{1}{2},\, \frac{3}{4}\right]$	[16,39]
13	$\left[\frac{3}{4},\, -x,\, 0\right]$	[17,24]
14	$\left[0,\, \frac{3}{4},\, -x\right]$	[18,21]
15	$\left[\frac{1}{2},\, \frac{3}{4},\, x\right]$	[19,47]
16	$\left[\frac{1}{4},\, x + \frac{1}{2},\, 0\right]$	[20,46]
17	$\left[\frac{3}{4},\, x,\, \frac{1}{2}\right]$	[22,44]
18	$\left[0,\, \frac{1}{4},\, x + \frac{1}{2}\right]$	[23,43]
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	$\left[\frac{1}{2} - x,\, \frac{1}{2},\, \frac{1}{4}\right]$	[37,38]
23	$\left[\frac{1}{4},\, \frac{1}{2} - x,\, \frac{1}{2}\right]$	[41,48]
24	$\left[\frac{1}{2},\, \frac{1}{4},\, \frac{1}{2} - x\right]$	[42,45]

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

No.	position	mapping
1	$\left[x,\, y,\, z\right]$	[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	$\left[z,\, x,\, y\right]$	[5]
6	$\left[y,\, z,\, x\right]$	[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]

continued …

Table 5

No.	position	mapping
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	$\left[-x, -y, -z\right]$	[13]
14	$\left[-x, y, z + \frac{1}{2}\right]$	[14]
15	$\left[x + \frac{1}{2}, -y, z\right]$	[15]
16	$\left[x, y + \frac{1}{2}, -z\right]$	[16]
17	$\left[-z, -x, -y\right]$	[17]
18	$\left[-y, -z, -x\right]$	[18]
19	$\left[y + \frac{1}{2}, -z, x\right]$	[19]
20	$\left[z, x + \frac{1}{2}, -y\right]$	[20]
21	$\left[y, z + \frac{1}{2}, -x\right]$	[21]
22	$\left[-z, x, y + \frac{1}{2}\right]$	[22]
23	$\left[-y, z, x + \frac{1}{2}\right]$	[23]
24	$\left[z + \frac{1}{2}, -x, y\right]$	[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	$\left[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[37]
38	$\left[\frac{1}{2} - x, y + \frac{1}{2}, z\right]$	[38]
39	$\left[x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[39]
40	$\left[x + \frac{1}{2}, y, \frac{1}{2} - z\right]$	[40]
41	$\left[\frac{1}{2} - z, \frac{1}{2} - x, \frac{1}{2} - y\right]$	[41]
42	$\left[\frac{1}{2} - y, \frac{1}{2} - z, \frac{1}{2} - x\right]$	[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	$\left[\frac{1}{2} - z, x + \frac{1}{2}, y\right]$	[46]
47	$\left[\frac{1}{2} - y, z + \frac{1}{2}, x\right]$	[47]
48	$\left[z, \frac{1}{2} - x, y + \frac{1}{2}\right]$	[48]