MSG No. 214.69 $I4'_132'$ [Type III, cubic]

Table 1: Wyckoff site: `8a`, site symmetry: `.32'`

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

Table 2: Wyckoff site: `8b`, site symmetry: `.32'`

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

Table 3: Wyckoff site: `12c`, site symmetry: `2.2'2'`

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

Table 4: Wyckoff site: `12d`, site symmetry: `2.2'2'`

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

Table 5: Wyckoff site: `16e`, 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	$\left[x + \frac{1}{4}, \frac{1}{4} - x, x + \frac{3}{4}\right]$	`[13,18,23]`
6	$\left[x + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{4} - x\right]$	`[14,15,19]`
7	$\left[\frac{1}{4} - x, x + \frac{3}{4}, x + \frac{1}{4}\right]$	`[16,17,21]`
8	$\left[\frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x\right]$	`[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	$\left[x + \frac{3}{4}, \frac{3}{4} - x, x + \frac{1}{4}\right]$	`[37,42,47]`
14	$\left[x + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - x\right]$	`[38,39,43]`
15	$\left[\frac{3}{4} - x, x + \frac{1}{4}, x + \frac{3}{4}\right]$	`[40,41,45]`
16	$\left[\frac{3}{4} - x, \frac{3}{4} - x, \frac{3}{4} - x\right]$	`[44,46,48]`

Table 6: Wyckoff site: `24f`, 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]`

continued ...

Table 6

No.	position	mapping
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	$\left[x+\frac{1}{4},\ 0,\ \frac{3}{4}\right]$	[13,38]
11	$\left[x+\frac{3}{4},\ \frac{1}{2},\ \frac{1}{4}\right]$	[14,37]
12	$\left[0,\ \frac{1}{4},\ \frac{1}{4}-x\right]$	[15,24]
13	$\left[0,\ \frac{3}{4},\ x+\frac{1}{4}\right]$	[16,47]
14	$\left[\frac{1}{4},\ x+\frac{3}{4},\ \frac{1}{2}\right]$	[17,43]
15	$\left[\frac{1}{4},\ \frac{1}{4}-x,\ 0\right]$	[18,20]
16	$\left[\frac{3}{4},\ x+\frac{1}{4},\ 0\right]$	[19,41]
17	$\left[\frac{1}{4}-x,\ 0,\ \frac{1}{4}\right]$	[21,22]
18	$\left[\frac{1}{2},\ \frac{1}{4},\ x+\frac{3}{4}\right]$	[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	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{3}{4}-x\right]$	[39,48]
23	$\left[\frac{3}{4},\ \frac{3}{4}-x,\ \frac{1}{2}\right]$	[42,44]
24	$\left[\frac{3}{4}-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	[45,46]

Table 7: Wyckoff site: 24g, site symmetry: ..2'

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

continued ...

Table 7

No.	position	mapping
22	$\left[y+\frac{1}{2},\, y+\frac{3}{4},\, \frac{5}{8}\right]$	[30,39]
23	$\left[\frac{1}{2}-y,\, \frac{3}{4}-y,\, \frac{5}{8}\right]$	[33,48]
24	$\left[\frac{3}{4}-y,\, \frac{5}{8},\, \frac{1}{2}-y\right]$	[36,44]

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

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

Table 9: Wyckoff site: 48i, 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]

continued ...

Table 9

No.	position	mapping
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	$\left[x+\frac{1}{4},\ \frac{1}{4}-z,\ y+\frac{3}{4}\right]$	[13]
14	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ \frac{1}{4}-y\right]$	[14]
15	$\left[z+\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{4}-x\right]$	[15]
16	$\left[\frac{1}{4}-z,\ y+\frac{3}{4},\ x+\frac{1}{4}\right]$	[16]
17	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[17]
18	$\left[y+\frac{1}{4},\ \frac{1}{4}-x,\ z+\frac{3}{4}\right]$	[18]
19	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}-z\right]$	[19]
20	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[20]
21	$\left[\frac{1}{4}-x,\ z+\frac{3}{4},\ y+\frac{1}{4}\right]$	[21]
22	$\left[\frac{1}{4}-x,\ \frac{1}{4}-z,\ \frac{1}{4}-y\right]$	[22]
23	$\left[z+\frac{1}{4},\ \frac{1}{4}-y,\ x+\frac{3}{4}\right]$	[23]
24	$\left[\frac{1}{4}-z,\ \frac{1}{4}-y,\ \frac{1}{4}-x\right]$	[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	$\left[x+\frac{3}{4},\ \frac{3}{4}-z,\ y+\frac{1}{4}\right]$	[37]
38	$\left[x+\frac{1}{4},\ z+\frac{3}{4},\ \frac{3}{4}-y\right]$	[38]
39	$\left[z+\frac{1}{4},\ y+\frac{3}{4},\ \frac{3}{4}-x\right]$	[39]
40	$\left[\frac{3}{4}-z,\ y+\frac{1}{4},\ x+\frac{3}{4}\right]$	[40]
41	$\left[\frac{3}{4}-y,\ x+\frac{1}{4},\ z+\frac{3}{4}\right]$	[41]
42	$\left[y+\frac{3}{4},\ \frac{3}{4}-x,\ z+\frac{1}{4}\right]$	[42]
43	$\left[y+\frac{1}{4},\ x+\frac{3}{4},\ \frac{3}{4}-z\right]$	[43]
44	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ \frac{3}{4}-z\right]$	[44]
45	$\left[\frac{3}{4}-x,\ z+\frac{1}{4},\ y+\frac{3}{4}\right]$	[45]
46	$\left[\frac{3}{4}-x,\ \frac{3}{4}-z,\ \frac{3}{4}-y\right]$	[46]
47	$\left[z+\frac{3}{4},\ \frac{3}{4}-y,\ x+\frac{1}{4}\right]$	[47]
48	$\left[\frac{3}{4}-z,\ \frac{3}{4}-y,\ \frac{3}{4}-x\right]$	[48]