MSG No. 214.67 $I4_132$ [Type I, cubic]

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

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

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

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

Table 3: Wyckoff site: 12c, site symmetry: 2.22

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

Table 4: Wyckoff site: `12d`, site symmetry: `2.22`

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

Table 5: Wyckoff site: `16e`, site symmetry: `.3.`

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

Table 6: Wyckoff site: `24f`, site symmetry: `2..`

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	`[1,8]`
2	$\left[x + \frac{1}{4}, 0, \frac{3}{4}\right]$	`[2,27]`
3	$\left[x + \frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[3,26]`
4	$\left[0, \frac{1}{4}, \frac{1}{4} - x\right]$	`[4,16]`
5	$\left[0, \frac{3}{4}, x + \frac{1}{4}\right]$	`[5,39]`

continued ...

Table 6

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

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

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

continued ...

Table 7

No.	position	mapping
22	$\left[\frac{5}{8},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[32,38]
23	$\left[\frac{3}{4}-y,\ \frac{5}{8},\ \frac{1}{2}-y\right]$	[36,48]
24	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{5}{8}\right]$	[40,45]

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

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

Table 9: Wyckoff site: 48i, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[x+\frac{1}{4},\ \frac{1}{4}-z,\ y+\frac{3}{4}\right]$	[2]
3	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ \frac{1}{4}-y\right]$	[3]
4	$\left[z+\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{4}-x\right]$	[4]
5	$\left[\frac{1}{4}-z,\ y+\frac{3}{4},\ x+\frac{1}{4}\right]$	[5]
6	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[6]
7	$\left[y+\frac{1}{4},\ \frac{1}{4}-x,\ z+\frac{3}{4}\right]$	[7]

continued ...

Table 9

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