MSG No. 213.66 P_I4_132 [Type IV, cubic]

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

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

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

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

Table 3: Wyckoff site: 12c, site symmetry: 2'.22'

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

Table 4: Wyckoff site: `12d`, site symmetry: `2'.22'`

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

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	$\left[x + \frac{1}{2}, \frac{1}{2} - x, -x\right]$	`[8,22,23]`
6	$\left[-x, x + \frac{1}{2}, \frac{1}{2} - x\right]$	`[9,19,24]`
7	$\left[\frac{1}{2} - x, -x, x + \frac{1}{2}\right]$	`[10,20,21]`
8	$\left[\frac{3}{4} - x, \frac{3}{4} - x, \frac{3}{4} - x\right]$	`[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	$\left[x, -x, \frac{1}{2} - x\right]$	`[32,46,47]`
14	$\left[\frac{1}{2} - x, x, -x\right]$	`[33,43,48]`
15	$\left[-x, \frac{1}{2} - x, x\right]$	`[34,44,45]`
16	$\left[\frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x\right]$	`[36,38,40]`

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

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

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	$\left[\frac{3}{8}, -y, y+\frac{3}{4}\right]$	[2,10]
3	$\left[\frac{7}{8}, y+\frac{1}{2}, \frac{1}{4}-y\right]$	[3,9]
4	$\left[y, y+\frac{1}{4}, \frac{1}{8}\right]$	[4,18]
5	$\left[-y, y+\frac{3}{4}, \frac{3}{8}\right]$	[5,19]
6	$\left[\frac{1}{4}-y, \frac{7}{8}, y+\frac{1}{2}\right]$	[6,20]
7	$\left[y+\frac{1}{4}, \frac{1}{8}, y\right]$	[7,17]
8	$\left[\frac{5}{8}, \frac{1}{2}-y, \frac{3}{4}-y\right]$	[8,14]
9	$\left[y+\frac{3}{4}, \frac{3}{8}, -y\right]$	[11,22]
10	$\left[\frac{3}{4}-y, \frac{5}{8}, \frac{1}{2}-y\right]$	[12,24]
11	$\left[y+\frac{1}{2}, \frac{1}{4}-y, \frac{7}{8}\right]$	[15,23]
12	$\left[\frac{1}{2}-y, \frac{3}{4}-y, \frac{5}{8}\right]$	[16,21]
13	$\left[\frac{5}{8}, y+\frac{1}{2}, y+\frac{3}{4}\right]$	[25,37]
14	$\left[\frac{7}{8}, \frac{1}{2}-y, y+\frac{1}{4}\right]$	[26,34]
15	$\left[\frac{3}{8}, y, \frac{3}{4}-y\right]$	[27,33]
16	$\left[y+\frac{1}{2}, y+\frac{3}{4}, \frac{5}{8}\right]$	[28,42]
17	$\left[\frac{1}{2}-y, y+\frac{1}{4}, \frac{7}{8}\right]$	[29,43]
18	$\left[\frac{3}{4}-y, \frac{3}{8}, y\right]$	[30,44]
19	$\left[y+\frac{3}{4}, \frac{5}{8}, y+\frac{1}{2}\right]$	[31,41]
20	$\left[\frac{1}{8}, -y, \frac{1}{4}-y\right]$	[32,38]
21	$\left[y+\frac{1}{4}, \frac{7}{8}, \frac{1}{2}-y\right]$	[35,46]

continued ...

Table 7

No.	position	mapping
22	$\left[\frac{1}{4}-y,\ \frac{1}{8},\ -y\right]$	[36,48]
23	$\left[y,\ \frac{3}{4}-y,\ \frac{3}{8}\right]$	[39,47]
24	$\left[-y,\ \frac{1}{4}-y,\ \frac{1}{8}\right]$	[40,45]

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

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

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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[8]
9	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[9]
10	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	[10]
11	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}-z\right]$	[11]
12	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ \frac{3}{4}-z\right]$	[12]
13	$\left[\frac{1}{4}-x,\ z+\frac{3}{4},\ y+\frac{1}{4}\right]$	[13]
14	$\left[\frac{3}{4}-x,\ \frac{3}{4}-z,\ \frac{3}{4}-y\right]$	[14]
15	$\left[z+\frac{1}{4},\ \frac{1}{4}-y,\ x+\frac{3}{4}\right]$	[15]
16	$\left[\frac{3}{4}-z,\ \frac{3}{4}-y,\ \frac{3}{4}-x\right]$	[16]
17	$[z,\ x,\ y]$	[17]
18	$[y,\ z,\ x]$	[18]
19	$\left[-y,\ z+\frac{1}{2},\ \frac{1}{2}-x\right]$	[19]
20	$\left[\frac{1}{2}-z,\ -x,\ y+\frac{1}{2}\right]$	[20]
21	$\left[\frac{1}{2}-y,\ -z,\ x+\frac{1}{2}\right]$	[21]
22	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ -y\right]$	[22]
23	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ -x\right]$	[23]
24	$\left[-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[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	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	[32]
33	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[33]
34	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	[34]
35	$\left[y+\frac{1}{4},\ x+\frac{3}{4},\ \frac{3}{4}-z\right]$	[35]
36	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[36]
37	$\left[\frac{3}{4}-x,\ z+\frac{1}{4},\ y+\frac{3}{4}\right]$	[37]
38	$\left[\frac{1}{4}-x,\ \frac{1}{4}-z,\ \frac{1}{4}-y\right]$	[38]
39	$\left[z+\frac{3}{4},\ \frac{3}{4}-y,\ x+\frac{1}{4}\right]$	[39]
40	$\left[\frac{1}{4}-z,\ \frac{1}{4}-y,\ \frac{1}{4}-x\right]$	[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	$\left[\frac{1}{2}-y,\ z,\ -x\right]$	[43]
44	$\left[-z,\ \frac{1}{2}-x,\ y\right]$	[44]
45	$\left[-y,\ \frac{1}{2}-z,\ x\right]$	[45]
46	$\left[z,\ -x,\ \frac{1}{2}-y\right]$	[46]
47	$\left[y,\ -z,\ \frac{1}{2}-x\right]$	[47]
48	$\left[\frac{1}{2}-z,\ x,\ -y\right]$	[48]