MSG No. 122.338 $\quad I_c\bar{4}2d$ [Type IV, tetragonal]

Table 1: Wyckoff site: 8a, site symmetry: -4..

No.	position	mapping
1	$[0, 0, 0]$	[1,4,5,6]
2	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[2,3,7,8]
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[9,12,13,14]
4	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[10,11,15,16]
5	$\left[0, 0, \frac{1}{2}\right]$	[17,20,21,22]
6	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[18,19,23,24]
7	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[25,28,29,30]
8	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[26,27,31,32]

Table 2: Wyckoff site: 8b, site symmetry: -4'..

No.	position	mapping
1	$\left[0, 0, \frac{1}{4}\right]$	[1,4,21,22]
2	$\left[0, \frac{1}{2}, 0\right]$	[2,3,23,24]
3	$\left[0, 0, \frac{3}{4}\right]$	[5,6,17,20]
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[7,8,18,19]
5	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[9,12,29,30]
6	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[10,11,31,32]
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[13,14,25,28]
8	$\left[\frac{1}{2}, 0, 0\right]$	[15,16,26,27]

Table 3: Wyckoff site: 8c, site symmetry: 2'22'.

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{8}\right]$	[1,2,27,28]
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{8}\right]$	[3,4,25,26]
3	$\left[\frac{1}{4}, \frac{1}{4}, \frac{7}{8}\right]$	[5,15,24,30]
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{7}{8}\right]$	[6,16,23,29]
5	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{8}\right]$	[7,13,22,32]
6	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{8}\right]$	[8,14,21,31]
7	$\left[\frac{1}{4}, \frac{3}{4}, \frac{5}{8}\right]$	[9,10,19,20]
8	$\left[\frac{3}{4}, \frac{1}{4}, \frac{5}{8}\right]$	[11,12,17,18]

Table 4: Wyckoff site: 8d, site symmetry: 2'2'2.

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{8}\right]$	[1,11,18,28]
2	$\left[\frac{3}{4}, \frac{1}{4}, \frac{7}{8}\right]$	[2,12,17,27]
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{7}{8}\right]$	[3,9,20,26]
4	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{8}\right]$	[4,10,19,25]
5	$\left[\frac{1}{4}, \frac{1}{4}, \frac{5}{8}\right]$	[5,8,30,31]
6	$\left[\frac{3}{4}, \frac{3}{4}, \frac{5}{8}\right]$	[6,7,29,32]
7	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{8}\right]$	[13,16,22,23]
8	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{8}\right]$	[14,15,21,24]

Table 5: Wyckoff site: 16e, site symmetry: 2...

No.	position	mapping
1	$[0, 0, z]$	[1,4]
2	$\left[0, \frac{1}{2}, \frac{1}{4} - z\right]$	[2,3]
3	$[0, 0, -z]$	[5,6]
4	$\left[0, \frac{1}{2}, z + \frac{1}{4}\right]$	[7,8]
5	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[9,12]
6	$\left[\frac{1}{2}, 0, \frac{3}{4} - z\right]$	[10,11]
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	[13,14]
8	$\left[\frac{1}{2}, 0, z + \frac{3}{4}\right]$	[15,16]
9	$\left[0, 0, z + \frac{1}{2}\right]$	[17,20]
10	$\left[0, \frac{1}{2}, \frac{3}{4} - z\right]$	[18,19]
11	$\left[0, 0, \frac{1}{2} - z\right]$	[21,22]
12	$\left[0, \frac{1}{2}, z + \frac{3}{4}\right]$	[23,24]
13	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[25,28]
14	$\left[\frac{1}{2}, 0, \frac{1}{4} - z\right]$	[26,27]
15	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[29,30]
16	$\left[\frac{1}{2}, 0, z + \frac{1}{4}\right]$	[31,32]

Table 6: Wyckoff site: 16f, site symmetry: .2.

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{1}{8}\right]$	[1,2]
2	$\left[-x, \frac{3}{4}, \frac{1}{8}\right]$	[3,4]
3	$\left[\frac{1}{4}, -x, \frac{7}{8}\right]$	[5,15]
4	$\left[\frac{3}{4}, x, \frac{7}{8}\right]$	[6,16]
5	$\left[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{8}\right]$	[7,13]
6	$\left[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{8}\right]$	[8,14]
7	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{5}{8}\right]$	[9,10]
8	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{5}{8}\right]$	[11,12]
9	$\left[x, \frac{1}{4}, \frac{5}{8}\right]$	[17,18]

continued ...

Table 6

No.	position	mapping
10	$\left[-x, \frac{3}{4}, \frac{5}{8}\right]$	[19,20]
11	$\left[\frac{1}{4}, -x, \frac{3}{8}\right]$	[21,31]
12	$\left[\frac{3}{4}, x, \frac{3}{8}\right]$	[22,32]
13	$\left[\frac{3}{4}, \frac{1}{2}-x, \frac{7}{8}\right]$	[23,29]
14	$\left[\frac{1}{4}, x+\frac{1}{2}, \frac{7}{8}\right]$	[24,30]
15	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{1}{8}\right]$	[25,26]
16	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{1}{8}\right]$	[27,28]

Table 7: Wyckoff site: 16g, site symmetry: .2'.

No.	position	mapping
1	$\left[\frac{3}{4}, y, \frac{1}{8}\right]$	[1,27]
2	$\left[\frac{3}{4}, \frac{1}{2}-y, \frac{1}{8}\right]$	[2,28]
3	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{1}{8}\right]$	[3,25]
4	$\left[\frac{1}{4}, -y, \frac{1}{8}\right]$	[4,26]
5	$\left[y, \frac{1}{4}, \frac{7}{8}\right]$	[5,24]
6	$\left[-y, \frac{3}{4}, \frac{7}{8}\right]$	[6,23]
7	$\left[-y, \frac{3}{4}, \frac{3}{8}\right]$	[7,22]
8	$\left[y, \frac{1}{4}, \frac{3}{8}\right]$	[8,21]
9	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{5}{8}\right]$	[9,19]
10	$\left[\frac{1}{4}, -y, \frac{5}{8}\right]$	[10,20]
11	$\left[\frac{3}{4}, y, \frac{5}{8}\right]$	[11,17]
12	$\left[\frac{3}{4}, \frac{1}{2}-y, \frac{5}{8}\right]$	[12,18]
13	$\left[y+\frac{1}{2}, \frac{3}{4}, \frac{3}{8}\right]$	[13,32]
14	$\left[\frac{1}{2}-y, \frac{1}{4}, \frac{3}{8}\right]$	[14,31]
15	$\left[\frac{1}{2}-y, \frac{1}{4}, \frac{7}{8}\right]$	[15,30]
16	$\left[y+\frac{1}{2}, \frac{3}{4}, \frac{7}{8}\right]$	[16,29]

Table 8: Wyckoff site: 16h, site symmetry: 2'..

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	[1,28]
2	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}-z\right]$	[2,27]
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}-z\right]$	[3,26]
4	$\left[\frac{1}{4}, \frac{3}{4}, z\right]$	[4,25]
5	$\left[\frac{1}{4}, \frac{1}{4}, -z\right]$	[5,30]
6	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[6,29]
7	$\left[\frac{3}{4}, \frac{3}{4}, z+\frac{1}{4}\right]$	[7,32]
8	$\left[\frac{1}{4}, \frac{1}{4}, z+\frac{1}{4}\right]$	[8,31]
9	$\left[\frac{1}{4}, \frac{3}{4}, z+\frac{1}{2}\right]$	[9,20]
10	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}-z\right]$	[10,19]
11	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}-z\right]$	[11,18]

continued ...

Table 8

No.	position	mapping
12	$\left[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}\right]$	[12,17]
13	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	[13,22]
14	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z\right]$	[14,21]
15	$\left[\frac{1}{4}, \frac{1}{4}, z + \frac{3}{4}\right]$	[15,24]
16	$\left[\frac{3}{4}, \frac{3}{4}, z + \frac{3}{4}\right]$	[16,23]

Table 9: Wyckoff site: 32i, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$\left[x, \frac{1}{2} - y, \frac{1}{4} - z\right]$	[2]
3	$\left[-x, y + \frac{1}{2}, \frac{1}{4} - z\right]$	[3]
4	$[-x, -y, z]$	[4]
5	$[y, -x, -z]$	[5]
6	$[-y, x, -z]$	[6]
7	$\left[-y, \frac{1}{2} - x, z + \frac{1}{4}\right]$	[7]
8	$\left[y, x + \frac{1}{2}, z + \frac{1}{4}\right]$	[8]
9	$\left[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[9]
10	$\left[x + \frac{1}{2}, -y, \frac{3}{4} - z\right]$	[10]
11	$\left[\frac{1}{2} - x, y, \frac{3}{4} - z\right]$	[11]
12	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[12]
13	$\left[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z\right]$	[13]
14	$\left[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z\right]$	[14]
15	$\left[\frac{1}{2} - y, -x, z + \frac{3}{4}\right]$	[15]
16	$\left[y + \frac{1}{2}, x, z + \frac{3}{4}\right]$	[16]
17	$\left[x, y, z + \frac{1}{2}\right]$	[17]
18	$\left[x, \frac{1}{2} - y, \frac{3}{4} - z\right]$	[18]
19	$\left[-x, y + \frac{1}{2}, \frac{3}{4} - z\right]$	[19]
20	$\left[-x, -y, z + \frac{1}{2}\right]$	[20]
21	$\left[y, -x, \frac{1}{2} - z\right]$	[21]
22	$\left[-y, x, \frac{1}{2} - z\right]$	[22]
23	$\left[-y, \frac{1}{2} - x, z + \frac{3}{4}\right]$	[23]
24	$\left[y, x + \frac{1}{2}, z + \frac{3}{4}\right]$	[24]
25	$\left[x + \frac{1}{2}, y + \frac{1}{2}, z\right]$	[25]
26	$\left[x + \frac{1}{2}, -y, \frac{1}{4} - z\right]$	[26]
27	$\left[\frac{1}{2} - x, y, \frac{1}{4} - z\right]$	[27]
28	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z\right]$	[28]
29	$\left[y + \frac{1}{2}, \frac{1}{2} - x, -z\right]$	[29]
30	$\left[\frac{1}{2} - y, x + \frac{1}{2}, -z\right]$	[30]
31	$\left[\frac{1}{2} - y, -x, z + \frac{1}{4}\right]$	[31]
32	$\left[y + \frac{1}{2}, x, z + \frac{1}{4}\right]$	[32]