MSG No. 142.569 $I4_1/a'c'd'$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: `8b`, site symmetry: `2.22`

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

Table 3: Wyckoff site: `16c`, site symmetry: `-1'`

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[24,32]`

Table 4: Wyckoff site: `16d`, site symmetry: `2..`

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

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

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

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

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

Table 7: Wyckoff site: `32g`, site symmetry: `1`

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

continued ...

Table 7

No.	position	mapping
24	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ \frac{3}{4}-z\right]$	[24]
25	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[25]
26	$\left[y+\frac{1}{4},\ \frac{3}{4}-x,\ \frac{1}{4}-z\right]$	[26]
27	$\left[\frac{3}{4}-y,\ x+\frac{3}{4},\ \frac{1}{4}-z\right]$	[27]
28	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[28]
29	$\left[x+\frac{1}{2},\ -y,\ z\right]$	[29]
30	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ z+\frac{3}{4}\right]$	[31]
32	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[32]