MSG No. 142.568 $I4_1'/a'cd'$ [Type III, tetragonal]

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

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

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

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

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

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[20,32]

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

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

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

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

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

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

continued ...

Table 7

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