MSG No. 142.563 $I4_1/a'cd$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: `8b`, site symmetry: `2.2'2'`

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

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

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[24,28]`

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

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

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

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

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

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

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	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	`[4]`
5	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	`[5]`
6	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[6]`
7	$\left[\frac{3}{4}-y,\ \frac{1}{4}-x,\ z+\frac{1}{4}\right]$	`[7]`
8	$\left[y+\frac{1}{4},\ x+\frac{1}{4},\ z+\frac{1}{4}\right]$	`[8]`
9	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	`[9]`
10	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	`[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	$[-x,\ -y,\ -z]$	`[13]`
14	$\left[y+\frac{3}{4},\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	`[14]`
15	$\left[\frac{1}{4}-y,\ x+\frac{1}{4},\ \frac{3}{4}-z\right]$	`[15]`
16	$\left[x,\ y+\frac{1}{2},\ -z\right]$	`[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	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	`[20]`
21	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	`[21]`
22	$\left[x+\frac{1}{2},\ -y,\ z\right]$	`[22]`
23	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ z+\frac{3}{4}\right]$	`[23]`

continued ...

Table 7

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