MSG No. 142.565 $I4_1'/acd'$ [Type III, tetragonal]

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

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

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	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{7}{8}\right]$	`[2,3,25,26]`
3	$\left[0,\ \frac{3}{4},\ \frac{7}{8}\right]$	`[5,8,31,32]`
4	$\left[0,\ \frac{1}{4},\ \frac{5}{8}\right]$	`[6,7,13,14]`
5	$\left[0,\ \frac{3}{4},\ \frac{3}{8}\right]$	`[9,10,18,19]`
6	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{3}{8}\right]$	`[15,16,21,24]`
7	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{5}{8}\right]$	`[17,20,27,28]`
8	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{1}{8}\right]$	`[22,23,29,30]`

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

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[28,32]

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

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

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	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	`[2,26]`
3	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	`[3,25]`
4	$\left[-x,\ \frac{1}{4}-x,\ \frac{1}{8}\right]$	`[4,12]`
5	$\left[-x,\ \frac{3}{4}-x,\ \frac{7}{8}\right]$	`[5,31]`
6	$\left[-x,\ x+\frac{1}{4},\ \frac{5}{8}\right]$	`[6,14]`
7	$\left[x,\ \frac{1}{4}-x,\ \frac{5}{8}\right]$	`[7,13]`
8	$\left[x,\ x+\frac{3}{4},\ \frac{7}{8}\right]$	`[8,32]`
9	$\left[-x,\ x+\frac{3}{4},\ \frac{3}{8}\right]$	`[9,19]`
10	$\left[x,\ \frac{3}{4}-x,\ \frac{3}{8}\right]$	`[10,18]`
11	$\left[\frac{1}{2}-x,\ \frac{1}{4}-x,\ \frac{3}{8}\right]$	`[15,21]`
12	$\left[x+\frac{1}{2},\ x+\frac{1}{4},\ \frac{3}{8}\right]$	`[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	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	`[22,30]`
16	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	`[23,29]`

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

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

continued ...

Table 7

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