MSG No. 142.564 $I4_1'/ac'd$ [Type III, tetragonal]

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

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

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

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

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

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

Table 3

No.	position	mapping
16	$\left[\frac{3}{4},\frac{3}{4},\frac{3}{4}\right]$	[20,24]

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	$\left[0,\frac{3}{4},-z\right]$	[5,6]
4	$\left[\frac{1}{2},\frac{1}{4},z+\frac{1}{4}\right]$	[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	$\left[0,\frac{1}{4},\frac{3}{4}-z\right]$	[13,14]
8	$\left[0,\frac{1}{4},z+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2},\frac{1}{4},\frac{1}{2}-z\right]$	[21,22]
12	$\left[0,\frac{3}{4},z+\frac{3}{4}\right]$	[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	$\left[\frac{1}{2},\frac{3}{4},\frac{1}{4}-z\right]$	[29,30]
16	$\left[\frac{1}{2},\frac{3}{4},z\right]$	[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	$\left[-x,0,\frac{3}{4}\right]$	[5,15]
6	$\left[x,\frac{1}{2},\frac{3}{4}\right]$	[6,16]
7	$\left[\frac{3}{4},\frac{1}{4}-x,\frac{1}{2}\right]$	[7,13]
8	$\left[\frac{1}{4},x+\frac{1}{4},\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x,\frac{1}{2},\frac{1}{4}\right]$	[21,31]
14	$\left[x+\frac{1}{2},0,\frac{1}{4}\right]$	[22,32]
15	$\left[\frac{1}{4},\frac{3}{4}-x,0\right]$	[23,29]
16	$\left[\frac{3}{4},x+\frac{3}{4},0\right]$	[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	$\left[-x,\ \frac{3}{4}-x,\ \frac{7}{8}\right]$	[5,23]
4	$\left[x,\ x+\frac{3}{4},\ \frac{7}{8}\right]$	[6,24]
5	$\left[\frac{1}{2}-x,\ \frac{1}{4}-x,\ \frac{3}{8}\right]$	[7,21]
6	$\left[x+\frac{1}{2},\ x+\frac{1}{4},\ \frac{3}{8}\right]$	[8,22]
7	$\left[-x,\ x+\frac{3}{4},\ \frac{3}{8}\right]$	[9,28]
8	$\left[x,\ \frac{3}{4}-x,\ \frac{3}{8}\right]$	[10,27]
9	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	[11,26]
10	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ \frac{7}{8}\right]$	[12,25]
11	$\left[x,\ \frac{1}{4}-x,\ \frac{5}{8}\right]$	[13,16]
12	$\left[-x,\ x+\frac{1}{4},\ \frac{5}{8}\right]$	[14,15]
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	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	[29,32]
16	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ \frac{1}{8}\right]$	[30,31]

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

No.	position	mapping
1	$\left[x,\ y,\ z\right]$	[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	$\left[-x,\ -y,\ -z\right]$	[5]
6	$\left[x,\ y+\frac{1}{2},\ -z\right]$	[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	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[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	$\left[y+\frac{3}{4},\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[13]
14	$\left[\frac{1}{4}-y,\ x+\frac{1}{4},\ \frac{3}{4}-z\right]$	[14]
15	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	[15]
16	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[21]
22	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[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	$\left[\frac{3}{4} - y,\, x + \frac{1}{4},\, z + \frac{3}{4}\right]$	[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	$\left[y + \frac{1}{4},\, \frac{3}{4} - x,\, \frac{1}{4} - z\right]$	[29]
30	$\left[\frac{3}{4} - y,\, x + \frac{3}{4},\, \frac{1}{4} - z\right]$	[30]
31	$\left[\frac{1}{2} - x,\, y + \frac{1}{2},\, z\right]$	[31]
32	$\left[x + \frac{1}{2},\, -y,\, z\right]$	[32]

$\left[y + \frac{3}{4},\, x + \frac{3}{4},\, z + \frac{3}{4}\right]$

$\left[\frac{3}{4} - y,\, x + \frac{1}{4},\, z + \frac{3}{4}\right]$

$\left[y + \frac{1}{4},\, \frac{1}{4} - x,\, z + \frac{3}{4}\right]$

$\left[y + \frac{1}{4},\, \frac{3}{4} - x,\, \frac{1}{4} - z\right]$

$\left[\frac{3}{4} - y,\, x + \frac{3}{4},\, \frac{1}{4} - z\right]$