MSG No. 70.529 $Fd'dd$ [Type III, orthorhombic]

Table 1: Wyckoff site: `8a`, site symmetry: `22'2'`

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

Table 2: Wyckoff site: `8b`, site symmetry: `22'2'`

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

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

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[25,31]

Table 4: Wyckoff site: 16d, site symmetry: -1'

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

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

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

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

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

Table 7: Wyckoff site: `16g`, site symmetry: `..2'`

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

Table 8: Wyckoff site: `32h`, site symmetry: `1`

No.	position	mapping
1	$[x, y, z]$	`[1]`

continued ...

Table 8

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