MSG No. 70.527 $Fddd$ [Type I, orthorhombic]

Table 1: Wyckoff site: 8a, site symmetry: 222

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

Table 2: Wyckoff site: 8b, site symmetry: 222

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

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

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[25,29]

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

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

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	$\left[\frac{3}{4} - x, \frac{1}{8}, \frac{5}{8}\right]$	[3,12]
4	$\left[\frac{3}{4} - x, \frac{5}{8}, \frac{1}{8}\right]$	[4,11]
5	$\left[-x, \frac{7}{8}, \frac{7}{8}\right]$	[5,14]
6	$\left[-x, \frac{3}{8}, \frac{3}{8}\right]$	[6,13]
7	$\left[x + \frac{1}{4}, \frac{7}{8}, \frac{3}{8}\right]$	[7,16]
8	$\left[x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}\right]$	[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	$\left[\frac{1}{4} - x, \frac{1}{8}, \frac{1}{8}\right]$	[19,28]
12	$\left[\frac{1}{4} - x, \frac{5}{8}, \frac{5}{8}\right]$	[20,27]
13	$\left[\frac{1}{2} - x, \frac{7}{8}, \frac{3}{8}\right]$	[21,30]
14	$\left[\frac{1}{2} - x, \frac{3}{8}, \frac{7}{8}\right]$	[22,29]
15	$\left[x + \frac{3}{4}, \frac{7}{8}, \frac{7}{8}\right]$	[23,32]
16	$\left[x + \frac{3}{4}, \frac{3}{8}, \frac{3}{8}\right]$	[24,31]

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

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

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

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

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	$\left[\frac{3}{4}-x,\ y,\ \frac{3}{4}-z\right]$	[3]
4	$\left[\frac{3}{4}-x,\ \frac{3}{4}-y,\ z\right]$	[4]
5	$[-x,\ -y,\ -z]$	[5]
6	$\left[-x,\ y+\frac{1}{4},\ z+\frac{1}{4}\right]$	[6]
7	$\left[x+\frac{1}{4},\ -y,\ z+\frac{1}{4}\right]$	[7]
8	$\left[x+\frac{1}{4},\ y+\frac{1}{4},\ -z\right]$	[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	$\left[\frac{3}{4}-x,\ y+\frac{1}{2},\ \frac{1}{4}-z\right]$	[11]
12	$\left[\frac{3}{4}-x,\ \frac{1}{4}-y,\ z+\frac{1}{2}\right]$	[12]
13	$\left[-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[13]
14	$\left[-x,\ y+\frac{3}{4},\ z+\frac{3}{4}\right]$	[14]
15	$\left[x+\frac{1}{4},\ \frac{1}{2}-y,\ z+\frac{3}{4}\right]$	[15]
16	$\left[x+\frac{1}{4},\ y+\frac{3}{4},\ \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{4}-x,\ y,\ \frac{1}{4}-z\right]$	[19]
20	$\left[\frac{1}{4}-x,\ \frac{3}{4}-y,\ z+\frac{1}{2}\right]$	[20]
21	$\left[\frac{1}{2}-x,\ -y,\ \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x,\ y+\frac{1}{4},\ z+\frac{3}{4}\right]$	[22]
23	$\left[x+\frac{3}{4},\ -y,\ z+\frac{3}{4}\right]$	[23]
24	$\left[x+\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{4}-x,\ y+\frac{1}{2},\ \frac{3}{4}-z\right]$	[27]
28	$\left[\frac{1}{4}-x,\ \frac{1}{4}-y,\ z\right]$	[28]
29	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	[29]
30	$\left[\frac{1}{2}-x,\ y+\frac{3}{4},\ z+\frac{1}{4}\right]$	[30]
31	$\left[x+\frac{3}{4},\ \frac{1}{2}-y,\ z+\frac{1}{4}\right]$	[31]
32	$\left[x+\frac{3}{4},\ y+\frac{3}{4},\ -z\right]$	[32]