MSG No. 70.528 $Fddd1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: `8a`, site symmetry: `2221'`

No.	position	mapping
1	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}\right]$	`[1,10,19,28,33,42,51,60]`
2	$\left[\frac{1}{8}, \frac{5}{8}, \frac{5}{8}\right]$	`[2,9,20,27,34,41,52,59]`
3	$\left[\frac{5}{8}, \frac{1}{8}, \frac{5}{8}\right]$	`[3,12,17,26,35,44,49,58]`
4	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{8}\right]$	`[4,11,18,25,36,43,50,57]`
5	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	`[5,14,23,32,37,46,55,64]`
6	$\left[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}\right]$	`[6,13,24,31,38,45,56,63]`
7	$\left[\frac{3}{8}, \frac{7}{8}, \frac{3}{8}\right]$	`[7,16,21,30,39,48,53,62]`
8	$\left[\frac{3}{8}, \frac{3}{8}, \frac{7}{8}\right]$	`[8,15,22,29,40,47,54,61]`

Table 2: Wyckoff site: `8b`, site symmetry: `2221'`

No.	position	mapping
1	$\left[\frac{1}{8}, \frac{1}{8}, \frac{5}{8}\right]$	`[1,10,19,28,33,42,51,60]`
2	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	`[2,9,20,27,34,41,52,59]`
3	$\left[\frac{5}{8}, \frac{1}{8}, \frac{1}{8}\right]$	`[3,12,17,26,35,44,49,58]`
4	$\left[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}\right]$	`[4,11,18,25,36,43,50,57]`
5	$\left[\frac{7}{8}, \frac{7}{8}, \frac{3}{8}\right]$	`[5,14,23,32,37,46,55,64]`
6	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	`[6,13,24,31,38,45,56,63]`
7	$\left[\frac{3}{8}, \frac{7}{8}, \frac{7}{8}\right]$	`[7,16,21,30,39,48,53,62]`
8	$\left[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}\right]$	`[8,15,22,29,40,47,54,61]`

Table 3: Wyckoff site: `16c`, site symmetry: `-11'`

No.	position	mapping
1	$[0, 0, 0]$	`[1,5,33,37]`
2	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	`[2,14,34,46]`
3	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	`[3,23,35,55]`
4	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	`[4,32,36,64]`
5	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	`[6,10,38,42]`
6	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	`[7,19,39,51]`
7	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	`[8,28,40,60]`
8	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[9,13,41,45]`
9	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[11,31,43,63]`
10	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[12,24,44,56]`
11	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	`[15,27,47,59]`
12	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[16,20,48,52]`
13	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[17,21,49,53]`
14	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	`[18,30,50,62]`
15	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	`[22,26,54,58]`

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[25,29,57,61]`

Table 4: Wyckoff site: `16d`, site symmetry: `-11'`

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1,5,33,37]`
2	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	`[2,14,34,46]`
3	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	`[3,23,35,55]`
4	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	`[4,32,36,64]`
5	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	`[6,10,38,42]`
6	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	`[7,19,39,51]`
7	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	`[8,28,40,60]`
8	$\left[\frac{1}{2}, 0, 0\right]$	`[9,13,41,45]`
9	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	`[11,31,43,63]`
10	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	`[12,24,44,56]`
11	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	`[15,27,47,59]`
12	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	`[16,20,48,52]`
13	$\left[0, \frac{1}{2}, 0\right]$	`[17,21,49,53]`
14	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	`[18,30,50,62]`
15	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	`[22,26,54,58]`
16	$\left[0, 0, \frac{1}{2}\right]$	`[25,29,57,61]`

Table 5: Wyckoff site: `16e`, site symmetry: `2..1'`

No.	position	mapping
1	$\left[x, \frac{1}{8}, \frac{1}{8}\right]$	`[1,10,33,42]`
2	$\left[x, \frac{5}{8}, \frac{5}{8}\right]$	`[2,9,34,41]`
3	$\left[\frac{3}{4}-x, \frac{1}{8}, \frac{5}{8}\right]$	`[3,12,35,44]`
4	$\left[\frac{3}{4}-x, \frac{5}{8}, \frac{1}{8}\right]$	`[4,11,36,43]`
5	$\left[-x, \frac{7}{8}, \frac{7}{8}\right]$	`[5,14,37,46]`
6	$\left[-x, \frac{3}{8}, \frac{3}{8}\right]$	`[6,13,38,45]`
7	$\left[x+\frac{1}{4}, \frac{7}{8}, \frac{3}{8}\right]$	`[7,16,39,48]`
8	$\left[x+\frac{1}{4}, \frac{3}{8}, \frac{7}{8}\right]$	`[8,15,40,47]`
9	$\left[x+\frac{1}{2}, \frac{1}{8}, \frac{5}{8}\right]$	`[17,26,49,58]`
10	$\left[x+\frac{1}{2}, \frac{5}{8}, \frac{1}{8}\right]$	`[18,25,50,57]`
11	$\left[\frac{1}{4}-x, \frac{1}{8}, \frac{1}{8}\right]$	`[19,28,51,60]`
12	$\left[\frac{1}{4}-x, \frac{5}{8}, \frac{5}{8}\right]$	`[20,27,52,59]`
13	$\left[\frac{1}{2}-x, \frac{7}{8}, \frac{3}{8}\right]$	`[21,30,53,62]`
14	$\left[\frac{1}{2}-x, \frac{3}{8}, \frac{7}{8}\right]$	`[22,29,54,61]`
15	$\left[x+\frac{3}{4}, \frac{7}{8}, \frac{7}{8}\right]$	`[23,32,55,64]`
16	$\left[x+\frac{3}{4}, \frac{3}{8}, \frac{3}{8}\right]$	`[24,31,56,63]`

Table 6: Wyckoff site: `16f`, site symmetry: `.2.1'`

No.	position	mapping
1	$\left[\frac{1}{8}, y, \frac{1}{8}\right]$	`[1,19,33,51]`
2	$\left[\frac{1}{8}, \frac{3}{4}-y, \frac{5}{8}\right]$	`[2,20,34,52]`
3	$\left[\frac{5}{8}, y, \frac{5}{8}\right]$	`[3,17,35,49]`
4	$\left[\frac{5}{8}, \frac{3}{4}-y, \frac{1}{8}\right]$	`[4,18,36,50]`
5	$\left[\frac{7}{8}, -y, \frac{7}{8}\right]$	`[5,23,37,55]`
6	$\left[\frac{7}{8}, y+\frac{1}{4}, \frac{3}{8}\right]$	`[6,24,38,56]`
7	$\left[\frac{3}{8}, -y, \frac{3}{8}\right]$	`[7,21,39,53]`
8	$\left[\frac{3}{8}, y+\frac{1}{4}, \frac{7}{8}\right]$	`[8,22,40,54]`
9	$\left[\frac{1}{8}, y+\frac{1}{2}, \frac{5}{8}\right]$	`[9,27,41,59]`
10	$\left[\frac{1}{8}, \frac{1}{4}-y, \frac{1}{8}\right]$	`[10,28,42,60]`
11	$\left[\frac{5}{8}, y+\frac{1}{2}, \frac{1}{8}\right]$	`[11,25,43,57]`
12	$\left[\frac{5}{8}, \frac{1}{4}-y, \frac{5}{8}\right]$	`[12,26,44,58]`
13	$\left[\frac{7}{8}, \frac{1}{2}-y, \frac{3}{8}\right]$	`[13,31,45,63]`
14	$\left[\frac{7}{8}, y+\frac{3}{4}, \frac{7}{8}\right]$	`[14,32,46,64]`
15	$\left[\frac{3}{8}, \frac{1}{2}-y, \frac{7}{8}\right]$	`[15,29,47,61]`
16	$\left[\frac{3}{8}, y+\frac{3}{4}, \frac{3}{8}\right]$	`[16,30,48,62]`

Table 7: Wyckoff site: `16g`, site symmetry: `..21'`

No.	position	mapping
1	$\left[\frac{1}{8}, \frac{1}{8}, z\right]$	`[1,28,33,60]`
2	$\left[\frac{1}{8}, \frac{5}{8}, \frac{3}{4}-z\right]$	`[2,27,34,59]`
3	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{4}-z\right]$	`[3,26,35,58]`
4	$\left[\frac{5}{8}, \frac{5}{8}, z\right]$	`[4,25,36,57]`
5	$\left[\frac{7}{8}, \frac{7}{8}, -z\right]$	`[5,32,37,64]`
6	$\left[\frac{7}{8}, \frac{3}{8}, z+\frac{1}{4}\right]$	`[6,31,38,63]`
7	$\left[\frac{3}{8}, \frac{7}{8}, z+\frac{1}{4}\right]$	`[7,30,39,62]`
8	$\left[\frac{3}{8}, \frac{3}{8}, -z\right]$	`[8,29,40,61]`
9	$\left[\frac{1}{8}, \frac{5}{8}, z+\frac{1}{2}\right]$	`[9,20,41,52]`
10	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{4}-z\right]$	`[10,19,42,51]`
11	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{4}-z\right]$	`[11,18,43,50]`
12	$\left[\frac{5}{8}, \frac{1}{8}, z+\frac{1}{2}\right]$	`[12,17,44,49]`
13	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{2}-z\right]$	`[13,24,45,56]`
14	$\left[\frac{7}{8}, \frac{7}{8}, z+\frac{3}{4}\right]$	`[14,23,46,55]`
15	$\left[\frac{3}{8}, \frac{3}{8}, z+\frac{3}{4}\right]$	`[15,22,47,54]`
16	$\left[\frac{3}{8}, \frac{7}{8}, \frac{1}{2}-z\right]$	`[16,21,48,53]`

Table 8: Wyckoff site: `32h`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	`[1,33]`

continued ...

Table 8

No.	position	mapping
2	$\left[x,\ \frac{3}{4}-y,\ \frac{3}{4}-z\right]$	[2,34]
3	$\left[\frac{3}{4}-x,\ y,\ \frac{3}{4}-z\right]$	[3,35]
4	$\left[\frac{3}{4}-x,\ \frac{3}{4}-y,\ z\right]$	[4,36]
5	$[-x,\ -y,\ -z]$	[5,37]
6	$\left[-x,\ y+\frac{1}{4},\ z+\frac{1}{4}\right]$	[6,38]
7	$\left[x+\frac{1}{4},\ -y,\ z+\frac{1}{4}\right]$	[7,39]
8	$\left[x+\frac{1}{4},\ y+\frac{1}{4},\ -z\right]$	[8,40]
9	$\left[x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[9,41]
10	$\left[x,\ \frac{1}{4}-y,\ \frac{1}{4}-z\right]$	[10,42]
11	$\left[\frac{3}{4}-x,\ y+\frac{1}{2},\ \frac{1}{4}-z\right]$	[11,43]
12	$\left[\frac{3}{4}-x,\ \frac{1}{4}-y,\ z+\frac{1}{2}\right]$	[12,44]
13	$\left[-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[13,45]
14	$\left[-x,\ y+\frac{3}{4},\ z+\frac{3}{4}\right]$	[14,46]
15	$\left[x+\frac{1}{4},\ \frac{1}{2}-y,\ z+\frac{3}{4}\right]$	[15,47]
16	$\left[x+\frac{1}{4},\ y+\frac{3}{4},\ \frac{1}{2}-z\right]$	[16,48]
17	$\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[17,49]
18	$\left[x+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{1}{4}-z\right]$	[18,50]
19	$\left[\frac{1}{4}-x,\ y,\ \frac{1}{4}-z\right]$	[19,51]
20	$\left[\frac{1}{4}-x,\ \frac{3}{4}-y,\ z+\frac{1}{2}\right]$	[20,52]
21	$\left[\frac{1}{2}-x,\ -y,\ \frac{1}{2}-z\right]$	[21,53]
22	$\left[\frac{1}{2}-x,\ y+\frac{1}{4},\ z+\frac{3}{4}\right]$	[22,54]
23	$\left[x+\frac{3}{4},\ -y,\ z+\frac{3}{4}\right]$	[23,55]
24	$\left[x+\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{2}-z\right]$	[24,56]
25	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[25,57]
26	$\left[x+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{3}{4}-z\right]$	[26,58]
27	$\left[\frac{1}{4}-x,\ y+\frac{1}{2},\ \frac{3}{4}-z\right]$	[27,59]
28	$\left[\frac{1}{4}-x,\ \frac{1}{4}-y,\ z\right]$	[28,60]
29	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	[29,61]
30	$\left[\frac{1}{2}-x,\ y+\frac{3}{4},\ z+\frac{1}{4}\right]$	[30,62]
31	$\left[x+\frac{3}{4},\ \frac{1}{2}-y,\ z+\frac{1}{4}\right]$	[31,63]
32	$\left[x+\frac{3}{4},\ y+\frac{3}{4},\ -z\right]$	[32,64]