MSG No. 63.467 C_amcm [Type IV, orthorhombic]

Table 1: Wyckoff site: `8a`, site symmetry: `2/m..`

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

Table 2: Wyckoff site: `8b`, site symmetry: `2/m'..`

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

Table 3: Wyckoff site: `8c`, site symmetry: `2'/m..`

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

Table 4: Wyckoff site: `8d`, site symmetry: `2'/m'..`

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

Table 5: Wyckoff site: `8e`, site symmetry: `m2m`

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

Table 6: Wyckoff site: `8f`, site symmetry: `m'2'm`

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

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

No.	position	mapping
1	$[x, 0, 0]$	`[1,2]`
2	$\left[-x, 0, \frac{1}{2}\right]$	`[3,4]`
3	$[-x, 0, 0]$	`[5,6]`

continued ...

Table 7

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

Table 8: Wyckoff site: `16h`, site symmetry: `2'..`

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

Table 9: Wyckoff site: `16i`, site symmetry: `m..`

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,6]`
2	$[0,\ -y,\ -z]$	`[2,5]`
3	$\left[0,\ y,\ \frac{1}{2}-z\right]$	`[3,8]`
4	$\left[0,\ -y,\ z+\frac{1}{2}\right]$	`[4,7]`
5	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	`[9,14]`

continued ...

Table 9

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

Table 10: Wyckoff site: 16j, site symmetry: m'..

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

Table 11: Wyckoff site: 16k, site symmetry: ..m

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{4}\right]$	[1,8]
2	$\left[x,\ -y,\ \frac{3}{4}\right]$	[2,7]
3	$\left[-x,\ y,\ \frac{1}{4}\right]$	[3,6]
4	$\left[-x,\ -y,\ \frac{3}{4}\right]$	[4,5]
5	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[9,16]
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[10,15]
7	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[11,14]

continued ...

Table 11

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

Table 12: Wyckoff site: 321, site symmetry: 1

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

continued ...

Table 12

No.	position	mapping
32	$\left[x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[32]