MSG No. 64.480 C_Amca [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `mm'm'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `mm'm'`

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

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

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

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

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

Table 5: Wyckoff site: `8e`, site symmetry: `..2'/m'`

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

Table 6: Wyckoff site: `8f`, site symmetry: `2'22'`

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

Table 7: Wyckoff site: `8g`, site symmetry: `2m'm'`

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

Table 8: Wyckoff site: `8h`, site symmetry: `m2'm'`

No.	position	mapping
1	$[0, y, 0]$	`[1,6,27,32]`
2	$[0, -y, 0]$	`[2,5,28,31]`
3	$\left[\frac{1}{2}, y, \frac{1}{2}\right]$	`[3,8,25,30]`

continued ...

Table 8

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

Table 9: Wyckoff site: 8i, site symmetry: mm'2'

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

Table 10: Wyckoff site: 16j, site symmetry: ..2'

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

Table 11: Wyckoff site: `16k`, site symmetry: `.2.`

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

Table 12: Wyckoff site: `16l`, site symmetry: `2'..`

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

Table 13: Wyckoff site: `16m`, site symmetry: `m..`

No.	position	mapping
1	$[0, y, z]$	`[1,6]`

continued ...

Table 13

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

Table 14: Wyckoff site: `16n`, site symmetry: `.m'.`

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

Table 15: Wyckoff site: `16o`, site symmetry: `..m'`

No.	position	mapping
1	$[x,\, y,\, 0]$	`[1,32]`
2	$[x,\, -y,\, 0]$	`[2,31]`
3	$\left[\frac{1}{2} - x,\, y,\, \frac{1}{2}\right]$	`[3,30]`

continued ...

Table 15

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

Table 16: Wyckoff site: 32p, site symmetry: 1

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

continued ...

Table 16

No.	position	mapping
28	$[-x,\, -y,\, z]$	[28]
29	$\left[\frac{1}{2} - x,\, -y,\, \frac{1}{2} - z\right]$	[29]
30	$\left[\frac{1}{2} - x,\, y,\, z + \frac{1}{2}\right]$	[30]
31	$[x,\, -y,\, z]$	[31]
32	$[x,\, y,\, -z]$	[32]