MSG No. 72.546 I_cbam [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `m'm'm'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `m'm'm'`

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ 0\right]$	`[1,8,28,29]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[2,7,27,30]`

continued ...

Table 5

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

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

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

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

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

Table 8: Wyckoff site: 8h, site symmetry: 2m'm'

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	[1,2,23,24]
2	$\left[-x, 0, \frac{1}{4}\right]$	[3,4,21,22]
3	$\left[-x, 0, \frac{3}{4}\right]$	[5,6,19,20]
4	$\left[x, 0, \frac{3}{4}\right]$	[7,8,17,18]
5	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[9,10,31,32]

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[11,12,29,30]`
7	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[13,14,27,28]`
8	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{4}\right]$	`[15,16,25,26]`

Table 9: Wyckoff site: `8i`, site symmetry: `m'2'm`

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

Table 10: Wyckoff site: `8j`, site symmetry: `m'2m'`

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

Table 11: Wyckoff site: `8k`, site symmetry: `m'm'2`

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

Table 12: Wyckoff site: `8l`, site symmetry: `m'm'2`

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

Table 13: Wyckoff site: `16m`, site symmetry: `..2'`

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,22]`
2	$\left[0,\ -y,\ \frac{1}{2}-z\right]$	`[2,21]`
3	$\left[0,\ y,\ \frac{1}{2}-z\right]$	`[3,24]`
4	$[0,\ -y,\ z]$	`[4,23]`
5	$[0,\ -y,\ -z]$	`[5,18]`
6	$\left[0,\ y,\ z+\frac{1}{2}\right]$	`[6,17]`
7	$\left[0,\ -y,\ z+\frac{1}{2}\right]$	`[7,20]`
8	$[0,\ y,\ -z]$	`[8,19]`
9	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[9,30]`

continued ...

Table 14

No.	position	mapping
10	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	`[10,29]`
11	$\left[\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	`[11,32]`
12	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[12,31]`
13	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	`[13,26]`
14	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	`[14,25]`
15	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	`[15,28]`
16	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[16,27]`

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

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

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

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,8]`
2	$\left[x,\ -y,\ \frac{1}{2}\right]$	`[2,7]`
3	$\left[-x,\ y,\ \frac{1}{2}\right]$	`[3,6]`
4	$[-x,\ -y,\ 0]$	`[4,5]`
5	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[9,16]`
6	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	`[10,15]`
7	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	`[11,14]`
8	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[12,13]`
9	$\left[x,\ y,\ \frac{1}{2}\right]$	`[17,24]`
10	$[x,\ -y,\ 0]$	`[18,23]`
11	$[-x,\ y,\ 0]$	`[19,22]`

continued ...

Table 16

No.	position	mapping
12	$\left[-x,\, -y,\, \frac{1}{2}\right]$	[20,21]
13	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, 0\right]$	[25,32]
14	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[26,31]
15	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[27,30]
16	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, 0\right]$	[28,29]

Table 17: Wyckoff site: 16q, site symmetry: ..m'

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

Table 18: Wyckoff site: 32r, site symmetry: 1

No.	position	mapping
1	$[x,\, y,\, z]$	[1]
2	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	[2]
3	$\left[-x,\, y,\, \frac{1}{2}-z\right]$	[3]
4	$[-x,\, -y,\, z]$	[4]
5	$[-x,\, -y,\, -z]$	[5]
6	$\left[-x,\, y,\, z+\frac{1}{2}\right]$	[6]
7	$\left[x,\, -y,\, z+\frac{1}{2}\right]$	[7]
8	$[x,\, y,\, -z]$	[8]
9	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[9]
10	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[10]
11	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[11]
12	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[12]
13	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[13]

continued ...

Table 18

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