MSG No. 68.520 C_Acca [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[0, y, \frac{1}{4}\right]$	`[1,3,30,32]`
2	$\left[0, \frac{1}{2}-y, \frac{1}{4}\right]$	`[2,4,29,31]`
3	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{3}{4}\right]$	`[5,7,26,28]`

continued ...

Table 8

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ z]$	`[1,30]`

continued ...

Table 13

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

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

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

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

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{4}\right]$	[1,32]
2	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[2,31]
3	$\left[-x,\ y,\ \frac{1}{4}\right]$	[3,30]

continued ...

Table 15

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

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

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

continued ...

Table 16

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