MSG No. 68.518 C_ccca [Type IV, orthorhombic]

Table 1: Wyckoff site: `8a`, site symmetry: `2'2'2`

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

Table 2: Wyckoff site: `8b`, site symmetry: `222`

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{2},\ z\right]$	`[1,12,22,31]`
2	$\left[\frac{1}{4},\ 0,\ \frac{1}{2}-z\right]$	`[2,11,21,32]`
3	$\left[\frac{3}{4},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[3,10,24,29]`

continued ...

Table 7

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

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

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

Table 9: Wyckoff site: 16i, site symmetry: .2.

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

continued ...

Table 9

No.	position	mapping
14	$\left[\frac{1}{2}, -y, \frac{3}{4}\right]$	[26,28]
15	$\left[0, -y, \frac{1}{4}\right]$	[29,31]
16	$\left[0, y+\frac{1}{2}, \frac{1}{4}\right]$	[30,32]

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

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

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

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

continued ...

Table 11

No.	position	mapping
16	$\left[x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[31,32]

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

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

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

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

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

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

Table 15: Wyckoff site: 32o, 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	$\left[x, y, z+\frac{1}{2}\right]$	[17]
18	$\left[x, \frac{1}{2}-y, -z\right]$	[18]
19	$[-x, y, -z]$	[19]
20	$\left[-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[20]
21	$\left[\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x, y, z\right]$	[22]
23	$\left[x+\frac{1}{2}, \frac{1}{2}-y, z\right]$	[23]

continued ...

Table 15

No.	position	mapping
24	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[24]
25	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[25]
26	$\left[x+\frac{1}{2},\, -y,\, -z\right]$	[26]
27	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[27]
28	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[28]
29	$\left[-x,\, -y,\, \frac{1}{2}-z\right]$	[29]
30	$\left[-x,\, y+\frac{1}{2},\, z\right]$	[30]
31	$[x,\, -y,\, z]$	[31]
32	$\left[x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[32]