MSG No. 73.553 I_cbca [Type IV, orthorhombic]

Table 1: Wyckoff site: `8a`, site symmetry: `2'22'`

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

Table 2: Wyckoff site: `8b`, site symmetry: `22'2'`

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 7

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

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

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

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

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

continued ...

Table 9

No.	position	mapping
14	$\left[x,\ \frac{1}{2},\ \frac{1}{4}\right]$	[24,31]
15	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{4}\right]$	[25,26]
16	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	[29,30]

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

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

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

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

continued ...

Table 11

No.	position	mapping
16	$\left[\frac{3}{4}, y, \frac{1}{4}\right]$	[16,22]

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

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

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

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

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

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

Table 15: Wyckoff site: 32o, site symmetry: 1

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

continued ...

Table 15

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