MSG No. 74.561 I_cmma [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: `8g`, site symmetry: `mm2`

No.	position	mapping
1	$\left[0, \frac{1}{4}, z\right]$	`[1,4,6,7]`
2	$\left[0, \frac{3}{4}, -z\right]$	`[2,3,5,8]`
3	$\left[\frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}\right]$	`[9,12,14,15]`

continued ...

Table 7

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

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

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

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

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

continued ...

Table 9

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

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

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

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

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

continued ...

Table 11

No.	position	mapping
16	$\left[\frac{3}{4}, y, \frac{1}{2}\right]$	[16,22]

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

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

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

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

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

No.	position	mapping
1	$[x,\ y,\ z]$	`[1]`
2	$[x,\ -y,\ -z]$	`[2]`
3	$\left[-x,\ y+\frac{1}{2},\ -z\right]$	`[3]`
4	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	`[4]`
5	$[-x,\ -y,\ -z]$	`[5]`
6	$[-x,\ y,\ z]$	`[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	`[10]`
11	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	`[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	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[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	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	`[18]`
19	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[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	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	`[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	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[26]
27	$\left[\frac{1}{2}-x,\, y,\, -z\right]$	[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	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[30]
31	$\left[x+\frac{1}{2},\, -y,\, z\right]$	[31]
32	$\left[x+\frac{1}{2},\, y,\, -z\right]$	[32]