MSG No. 72.545 $Ib'a'm'$ [Type III, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `222`

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[1,2,3,4]`
2	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[5,6,7,8]`
3	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{3}{4}\right]$	`[9,10,11,12]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{4}\right]$	`[13,14,15,16]`

Table 2: Wyckoff site: `4b`, site symmetry: `222`

No.	position	mapping
1	$\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$	`[1,2,3,4]`
2	$\left[\frac{1}{2},\ 0,\ \frac{3}{4}\right]$	`[5,6,7,8]`
3	$\left[0,\ \frac{1}{2},\ \frac{3}{4}\right]$	`[9,10,11,12]`
4	$\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[13,14,15,16]`

Table 3: Wyckoff site: `4c`, site symmetry: `..2/m'`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,4,5,8]`
2	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[2,3,6,7]`
3	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[9,12,13,16]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[10,11,14,15]`

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

No.	position	mapping
1	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[1,4,5,8]`
2	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[2,3,6,7]`
3	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[9,12,13,16]`
4	$\left[0,\ \frac{1}{2},\ 0\right]$	`[10,11,14,15]`

Table 5: Wyckoff site: `8e`, site symmetry: `-1'`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,13]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[2,14]`

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[3,15]
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[4,16]
5	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[5,9]
6	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[6,10]
7	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[7,11]
8	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[8,12]

Table 6: Wyckoff site: 8f, site symmetry: 2..

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

Table 7: Wyckoff site: 8g, site symmetry: .2.

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

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

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

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$	`[10,11]`
7	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[13,16]`
8	$\left[\frac{1}{2},\ \frac{1}{2},\ z\right]$	`[14,15]`

Table 9: Wyckoff site: `8i`, site symmetry: `..2`

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,4]`
2	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[2,3]`
3	$\left[0,\ \frac{1}{2},\ -z\right]$	`[5,8]`
4	$\left[0,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[6,7]`
5	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[9,12]`
6	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[10,11]`
7	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[13,16]`
8	$\left[\frac{1}{2},\ 0,\ z\right]$	`[14,15]`

Table 10: Wyckoff site: `8j`, 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]`

Table 11: Wyckoff site: `16k`, 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]`

continued ...

Table 11

No.	position	mapping
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]
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]