MSG No. 72.540 $Ibam1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `2221'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2221'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `..2/m1'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `..2/m1'`

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

Table 5: Wyckoff site: `8e`, site symmetry: `-11'`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,13,17,29]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[2,14,18,30]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2..1'

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

Table 7: Wyckoff site: 8g, site symmetry: .2.1'

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

Table 8: Wyckoff site: 8h, site symmetry: ..21'

No.	position	mapping
1	$[0, 0, z]$	[1,4,17,20]
2	$\left[0, 0, \frac{1}{2}-z\right]$	[2,3,18,19]
3	$[0, 0, -z]$	[5,8,21,24]
4	$\left[0, 0, z+\frac{1}{2}\right]$	[6,7,22,23]
5	$\left[\frac{1}{2}, \frac{1}{2}, z+\frac{1}{2}\right]$	[9,12,25,28]

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[10,11,26,27]
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	[13,16,29,32]
8	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[14,15,30,31]

Table 9: Wyckoff site: 8i, site symmetry: ..21'

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

Table 10: Wyckoff site: 8j, site symmetry: ..m1'

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

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

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$\left[x, -y, \frac{1}{2} - z\right]$	[2,18]
3	$\left[-x, y, \frac{1}{2} - z\right]$	[3,19]
4	$[-x, -y, z]$	[4,20]
5	$[-x, -y, -z]$	[5,21]
6	$\left[-x, y, z + \frac{1}{2}\right]$	[6,22]
7	$\left[x, -y, z + \frac{1}{2}\right]$	[7,23]
8	$[x, y, -z]$	[8,24]

continued ...

Table 11

No.	position	mapping
9	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[9,25]
10	$\left[x+\frac{1}{2}, \frac{1}{2}-y, -z\right]$	[10,26]
11	$\left[\frac{1}{2}-x, y+\frac{1}{2}, -z\right]$	[11,27]
12	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[12,28]
13	$\left[\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[13,29]
14	$\left[\frac{1}{2}-x, y+\frac{1}{2}, z\right]$	[14,30]
15	$\left[x+\frac{1}{2}, \frac{1}{2}-y, z\right]$	[15,31]
16	$\left[x+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[16,32]