MSG No. 66.492 $Cccm1'$ [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	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{4}\right]$	`[9,10,11,12,25,26,27,28]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{3}{4}\right]$	`[13,14,15,16,29,30,31,32]`

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `..2/m1'`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ 0\right]$	`[1,8,12,13,17,24,28,29]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[2,7,11,14,18,23,27,30]`

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[3,6,10,15,19,22,26,31]
4	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[4,5,9,16,20,21,25,32]

Table 6: Wyckoff site: 4f, site symmetry: ..2/m1'

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

Table 7: Wyckoff site: 8g, 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	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[9,10,25,26]
6	$\left[\frac{1}{2}-x, \frac{1}{2}, \frac{1}{4}\right]$	[11,12,27,28]
7	$\left[\frac{1}{2}-x, \frac{1}{2}, \frac{3}{4}\right]$	[13,14,29,30]
8	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[15,16,31,32]

Table 8: Wyckoff site: 8h, 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	$\left[\frac{1}{2}, y+\frac{1}{2}, \frac{1}{4}\right]$	[9,11,25,27]
6	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{1}{4}\right]$	[10,12,26,28]
7	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{3}{4}\right]$	[13,15,29,31]
8	$\left[\frac{1}{2}, y+\frac{1}{2}, \frac{3}{4}\right]$	[14,16,30,32]

Table 9: Wyckoff site: `8i`, 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	$\left[\frac{1}{2},\ \frac{1}{2},\ z\right]$	`[9,12,25,28]`
6	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	`[10,11,26,27]`
7	$\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$	`[13,16,29,32]`
8	$\left[\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[14,15,30,31]`

Table 10: Wyckoff site: `8j`, 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	$\left[\frac{1}{2},\ 0,\ z\right]$	`[9,12,25,28]`
6	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	`[10,11,26,27]`
7	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[13,16,29,32]`
8	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[14,15,30,31]`

Table 11: Wyckoff site: `8k`, site symmetry: `..21'`

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

Table 12: Wyckoff site: `8l`, 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]`

continued ...

Table 12

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

Table 13: Wyckoff site: `16m`, 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]`
9	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	`[9,25]`
10	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	`[10,26]`
11	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[11,27]`
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	`[12,28]`
13	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	`[13,29]`
14	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[14,30]`
15	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[15,31]`
16	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	`[16,32]`